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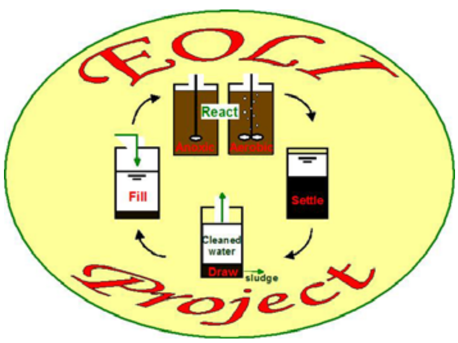
REPORT covering period from 1 November 2003 to 31 October 2004

Efficient Operation of Urban Wastewater Treatment Plant (EOLI)

Project homepage : http://www.auto.ucl.ac.be/EOLI/

Keywords : wastewater treatment (WWT), aerobic digestion, sequencing batch reactor (SBR), monitoring, control system



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TITLE : Efficient Operation of Urban Wastewater Treatment Plant (EOLI)

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Table of Contents

SUMMARY

UNAM:

Within WP5 UNAM studies the SBR dedicated to the treatment of wastewaters with toxic compounds. The design of the control software and instrumentation for a laboratory scale Sequencing Batch Reactors (SBR) was done in order to perform the first experiments defined by the EOLI protocol in WP1. The SBR was instrumented to measure Temperature, Dissolved Oxygen Concentration (DO) and Volume. Typical and new control strategies were tested, both in simulation and in laboratory experiments. After comparison, the Event Driven Time Optimal Control (EDTOC) strategy is proposed as a candidate to solve the given optimizing criteria for the given restrictions.

Advice and guidelines to design and to build a new field-scale SBR, now almost finished, were given to IBTECH.

1 SCIENTIFIC REPORT

1.1 Introduction

This report describes the progress of activities in WP5 for the EOLI project at UNAM. It includes a description of the methodology followed, activities conducted in the reporting period and outputs realised for the scientific work package involved.

At UNAM, the biodegradation of a toxic compound by naturally occurring microorganisms is investigated. In accordance with WP1 a laboratory-scale reactor was designed and assembled, early at the beginning of the project, to allow WP1,2 experiments to be conducted. Various control strategies were implemented including the traditional Fixed Time Control (FTC) and the new Event Driven Time Optimal Control (EDTOC).

A full introduction to the problem is given in the introductory sections of Annexes 01.WP5 and 04.WP5.

1.2 Methodology, activity and results of WP5

1.2.1. Methodology

A preliminary EM1 was used to develop simulators and first trial controllers for a laboratory-scale SBR. Different control strategies were proposed and tested both in simulation and in experiments with the laboratory-scale SBR.

The most promising strategy, the EDTOC, was studied also theoretically to evaluate its possibilities and its limitations.

A field scale reactor is been built to evaluate the EDTOC strategy with a mixture of real and synthetic wastewaters in a long term operation basis.

1.2.2. Activities

The problem formulation and justification was made. A full explanation is to be found in section 2 of Annex 03.WP5.

In the first year period a laboratory-scale pilot reactors was instrumented and the necessary control software developed. This was needed in order to allow WP1 to perform process experiments to provide experimental data to WP2 for parameter identification of the dynamical model. Section 4 of Annex 03.WP5 fully describes the laboratory-scale SBR.

By using a preliminary EM1 model a software simulator was designed to help operators to understand the effect, in the reactor's behavior, of parameter changes and uncertainties, mainly when using the typical Fixed Time Control (FTC) strategy.

Optimization objectives, associated problems, limitations and control variables were specified. An Observer Based Time Optimal Control (OBTOC) was studied using that same simulator designed for the FTC. Results were good in simulation but not as good in practice as the strategy was not robust against input perturbation (toxicant concentration peaks) nor against parameter uncertainties. Then a new idea was explored, the Event Driven Time Optimal Control (EDTOC). Such strategy replaces the normal Software-Sensor in the OBTOC with an Event-sensor which extracts from the system only the minimum necessary information for controlling it in a near optimal way. The tradeoff brings robustness to input perturbations and to model uncertainties. A new simulator was built using LabView, the same software used for real time control of the SBR, to study the EDTOC. Experiments later corroborated the advantages of the EDTOC over OBTOC and over FTC modes. The problem formulation and the description of the EDTOC strategy are given in sections 2 and 3 of Annex 01.WP5. A set of experiments using shock toxicant loads was performed by WP1 in order to evaluate the improvement of EDTOC operation over FTC. A full report is presented in Annex 11.WP5. Also, a general comparison of the FTC, the OBTOC and EDTOC is given in Annex 04.WP5.

Comparison with other possible strategy, the adaptive extremum seeking, was made for a whole class of bioreactors. Annex 05.WP5 describes in detail such comparison.

Advice and guidelines to design a field-scale SBR were given to IBTECH, in accordance with WP1, WP5, WP6 and WP8 personnel at UNAM. The reactor is now under construction.

Theoretical work is been done to evaluate the optimality, convergence and robustness of the EDTOC strategy and to find its limitations. Annex 02.WP5 describes in detail such theoretical approach.

1.2.3. Results

For the beginning of the second year the planned milestone was achieved. The one remaining milestone is not due until the middle of the third year:

- Tables summarizing optimization objectives, necessary control variables, and required hardware and software sensors. Expected economic savings, and improvement in process variables: **T0+12**
- Validation of optimal control law with real improvements in process and economic variables: **T0+30**

Deliverables are not due until the third year:

- D5.1 Control laws based on software sensors for optimising the performance of SBRs. **T0+27**
- D5.2 Report on full-scale performance of the adaptive optimal control law. **T0+30**

Table 3. Progress towards achieving objectives

WP5 Task & Objectives	Progress towards achieving objectives (Outputs)
Task 5.1 Specification of control variables and optimisation objectives	5.1.1 UNAM (10L and 1000L): Optimization objective is defined as treating the whole batch in the minimum possible time. Measured variable is Oxygen and Volume, the controlled variable is the biomass growth rate and the manipulated variable is the input inflow.
Task 5.2 Design of optimal and adaptive suboptimal control laws.	5.2.1 UNAM: A control law called Event Driven Time Optimal Control strategy (ED-TOC) was proposed and implemented. The ED-TOC strategy finds a variable, called gamma, related to the reaction rate. Such variable can be estimated in real time by using the dissolved oxygen in the reactor and its volume. The influent flow rate is controlled in such a manner that the biomass growth rate stays near to the maximal value. It is controlled maintaining the toxic concentration oscillating in a gap during the SBR filling. Every time it tries to leave this gap, an event is issued and the EDTOC then switches the influent flow on/off, to prevent it. This procedure will work regardless of the influent toxic concentration value and despite changes in most of the SBR parameters. Only the mass transfer coefficient and the dissolved oxygen concentration at saturation are needed to estimate gamma and they do not even need to be known precisely.
Task 5.3 Control law validation	5.3.1 UNAM: 3 different approaches to validation are taken. First simulation using both MATLAB and LABVIEW. Results are satisfactory. Second experimental tests. Results are also satisfactory. And third, theoretical proof of almost-optimality, convergence and robustness.
Task 5.4 Process improvement evaluation	5.4.1 UNAM: Single experimental batch tests have been made to evaluate process improvement. Annex 11.WP5 fully describes the improvements of EDTO over FTC. Long term tests are yet to be performed.

1.3 Problems encountered

No serious technical problems were encountered in the activities scheduled for the first two years of the project.

1.4 Publications and papers

1. Betancur, M.J.; Moreno, J.A. and Buitrón, G. (2004). Event-driven control for treating toxicants in aerobic sequencing batch bioreactors. *Proceedings of the 9th International Symposium on Computer Applications in Biotechnology (CAB9), CDROM file 1074*, 28-31 March 2004. Nancy, France.

2. Betancur, M.J.; Moreno J.A. and Buitrón, G. (2004). Practical Optimal Control For Fed-Batch Bioreactors. *Preprints of NOLCOS 2004 (Nonlinear Control Applications, Sep* 2004), pp 1517-1522, Stuttgart, Germany

3. Betancur, M.J; Titica, M; Moreno, J.A.; Dochain, D. and Guay, M. (2004). Event Software Sensor and Adaptive Extremum Seeking alternatives for optimizing a class of fed-batch bioreactors. *Proceedings of DYCOPS 2004*, Cambridge, Massachusetts, USA

4. Buitrón, G.; Moreno, J. A.; Betancur, M. J. and Moreno, I. (2004). Aerobic treatment of toxic wastewater: problems, solutions, and open questions. *Proceedings of the 3rd IWA Specialised Conference on Sequencing Batch Reactor Technology-SBR3*, 22-26 February 2004, Noosa, Australia

5. Buitrón, G.; Moreno-Andrade, I.; Betancur, M.J. and Moreno, J.A. (2004). Application of the event-driven time optimal control strategy for the degradation of inhibitory wastewater in a discontinuous bioreactor. *Proceedings in CD of the 4th World Water Congress, IWA.* 19-24/09/2004. Marrakech, Morocco, Paper ID 28156.

6. Buitrón, G.; Moreno-Andrade, I.; Betancur, M.J. and Moreno, J.A. (2004). Biodegradación de efluentes altamente contaminados por compuestos fenólicos utilizando una estrategia de control óptima, in Spanish. *Memorias del XIV Congreso de Ingeniería Ambiental y Ciencias Ambientales*. 12-14/05/2004, Mazatlán, México.

7. Moreno, J. and Dochain, D. Global observability and detectability analysis of uncertain reaction systems. *Submitted to the 10th. IFAC World Congress*. Prag, July 2005.

8. Betancur, M.J.; Moreno, J.A.; Moreno-Andrade, I. and Buitrón, G. Control strategies for treating toxic wastewater using bioreactors. *Submitted to the 10th. IFAC World Congress*. Prag, July 2005.

9. Betancur, M.J.; Moreno, J.A.; Buitrón, G. and Moreno-Andrade, I. Control y mejoras en biorreactores para tratar aguas residuales tóxicas, in Spanish. *Proceedings of the Congreso Anual de la AMCA*. October 2004, D.F., México, pp. 490-495.

1.5 Planning

Software modifications to the control software for the field-scale SBR are going to be prepared in order to allow integration with the supervision system.

After starting-up the field-scale SBR, evaluation and validation of the performance of the adaptative suboptimal control law will be made, in accordance with WP1.

Long-term running of the lab SBR to test the correctness of EDTOC strategy is going to be performed in accordance with WP1

2 MANAGEMENT REPORT

2.1 Meetings

Meetings with IBTECH and UNAM WP1, WP2 and WP6 participants were held when necessary, specially to give advice and guidelines for the design of the field scale pilot reactor by IBTECH.

2.2 Exchanges

One PhD students of UNAM was involved in exchanges at the end of first year until the beginning of the second one: Manuel BETANCUR has moved to CESAME/UCL (Louvain-la-Neuve, Belgium) since August 2003 to stay there for 6 months;

Prof. Jaime MORENO has visited CESAME-UCL in October 2003 for one week.

2.3 Problems

No management problems occurred in this period.

LIST OF ABBREVIATIONS

4CP	4-Chloro-Phenol
ASM	Activated Sludge Model
CESAME	Centre for Systems Engineering and Applied Mechanics
D1.x – D9.x	Deliverables
DO	Dissolved Oxygen Concentration
DSS	Decision Support System
EC	European Commission
EDTOC	Event Driven Time Optimal Control
EM1, 2	EOLI Model 1, 2
EOLI	Efficient Operation of Urban Wastewater Treatment Plant
FDI	Fault Detection and Isolation
FTC	Fixed Timing Control
GRADIENT	Groupe de Recherches et d'Animations pour le Développement, l'Innovation et l'Enseignement en Technologie
INCO	International Scientific Cooperation Projects
INRA	Institut National de la Recherche Agronomique
LBE	Laboratoire de Biotechnologie de l'Environnement
POLIMI	Politecnico di Milano
SBR	Sequencing Batch Reactor
SPES	Società di Progettazione Elettronica e Software
UCL	Université Catholique de Louvain
UNAM	Universidad Nacional Autónoma de México
UTC	Université Technologique de Compiègne
UU	Universidad de la República Oriental des Uruguay
WP	Work Package
WWTP	Wastewater Treatment Process

LIST OF ANNEXES

Annex 01.WP5 (paper)

Betancur, M.J.; Moreno, J. and Buitrón, G. (2004). Event-driven control for treating toxicants in aerobic sequencing batch bioreactors. *Proceedings of the 9th International Symposium on Computer Applications in Biotechnology (CAB9), CDROM file 1074*, 28-31 March 2004. Nancy, France.

Annex 02.WP5 (paper)

Betancur, M.J.; Moreno J.A. and Buitrón, G. (2004). Practical Optimal Control for Fed-Batch Bioreactors. *Preprints of NOLCOS 2004 (Nonlinear Control Applications, Sep* 2004), pp 1517-1522, Stuttgart, Germany

Annex 03.WP5 Mid-Term Partner6 (report)

Internal report prepared for the midterm meeting at LLN

Annex 04.WP5 (paper)

Buitrón, G.; Moreno, J. A.; Betancur, M. J. and Moreno, I. (2004). Aerobic treatment of toxic wastewater: problems, solutions, and open questions. *Proceedings of the 3rd IWA Specialised Conference on Sequencing Batch Reactor Technology-SBR3*, 22-26 February 2004, Noosa, Australia

Annex 05.WP5 (paper)

Betancur, M.J; Titica, M; Moreno, J.; Dochain, D. and Guay, M. (2004). Event Software Sensor and Adaptive Extremum Seeking alternatives for optimizing a class of fed-batch bioreactors. *Proceedings of DYCOPS 2004,* Cambridge, Massachusetts, USA

Annex 06.WP5 (paper)

Buitrón, G.; Moreno-Andrade, I.; Betancur, M.J. and Moreno, J.A. (2004). Application of the event-driven time optimal control strategy for the degradation of inhibitory wastewater in a discontinuous bioreactor. *Proceedings in CD of the 4th World Water Congress, IWA.* 19-24/09/2004. Marrakech, Morocco, Paper ID 28156.

Annex 07.WP5 (paper)

Buitrón, G.; Moreno-Andrade, I.; Betancur, M.J. and Moreno, J.A. (2004). Biodegradación de efluentes altamente contaminados por compuestos fenólicos utilizando una estrategia de control óptima, in Spanish. *Memorias del XIV Congreso de Ingeniería Ambiental y Ciencias Ambientales.* 12-14/05/2004, Mazatlán, México.

Annex 08.WP5 (paper)

Moreno, J. and Dochain, D. Global observability and detectability analysis of uncertain reaction systems. *Submitted to the 10th. IFAC World Congress*. Prag, July 2005.

Annex 09.WP5 (paper)

Betancur, M.J.; Moreno, J.A.; Moreno-Andrade, I. and Buitrón, G. Control strategies for treating toxic wastewater using bioreactors. *Submitted to the 10th. IFAC World Congress*. Prag, July 2005.

Annex 10.WP5 (paper)

Betancur, M.J.; Moreno, J.A.; Buitrón, G. and Moreno-Andrade, I. Control y mejoras en biorreactores para tratar aguas residuales tóxicas, in Spanish. *Proceedings of the Congreso Anual de la AMCA*. October 2004, D.F., México, pp. 490-495.

Annex 11.WP5 Improvement experiments

EVENT-DRIVEN CONTROL FOR TREATING TOXICANTS IN AEROBIC SEQUENCING BATCH BIOREACTORS

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Abstract: The use of sequencing batch bioreactors (SBR) for treating polluted wastewater is environmentally important. But the standard operation of SBRs is far from optimal when treating toxicants, because of the inhibition phenomena. The main technical problem is the lack of practical pollutant sensors. In this work an *event-driven time optimal control* (ED-TOC) is proposed to circumvent these problems. By measuring the dissolved oxygen and estimating some reaction rate events the ED-TOC maintains the pollutant concentration at optimal levels, and provides a robust, economical and an almost time-optimal operation mode.

Keywords: Control applications, Optimal control, Water pollution, Wastewater treatment.

1. INTRODUCTION

Industrial wastewater (WW) polluted with organic toxic substrates poses a real and difficult environmental problem, especially when intermittent industrial operation generates a sudden substrate amount increase (toxicant concentration peaks). Non-conventional processes, like the aerobic sequencing batch bioreactors (SBRs), may be used to treat such substrates, with satisfactory removal efficiency, if proper control methods are implemented. But usually that is not the case. Instead SBRs are commonly operated in an open loop *batch* mode that uses fixed timing for the filling, reaction, settling, draw and idle stages. Hence the SBR's cycle time and its efficiency could be improved by implementing some type of closed-loop control. But, as there exist no practical/economical toxicant substrate sensors for industrial use, the need for measuring the toxicant substrate either in the influent or inside the SBR should be avoided.

Several works have addressed this problem using dissolved oxygen (DO) concentration or carbon dioxide evolution rate to determine the end of the reaction stage. Sheppard and Cooper (1990) proposed a Self-Cycling Fermentation based on the correlation between DO and cellular respiration. The method has also been applied for treatment of Kraft process waters (Milet and Duff, 1998) and agro-industrial water (Nguyen *et al*., 2000). Moreno and Buitrón (1998) presented a *Time-Optimal Control* (TOC), based on DO measurements, such that the specific growth rate was maintained close to its maximum during the reaction period. Buitrón *et al.* (2001) used DO to sub-optimally asses the end of the reaction period in an otherwise standard batch SBR.

This work describes a new *Event-Driven* (ED) TOC strategy, based on DO measures, to robustly control the reaction rate of an aerobic SBR for treating toxicant substrates. The ED-TOC maintains the reaction rate oscillating around its maximum thus achieving almost time-optimality. This objective is reached even in the presence of uncertainty about the reactor's model and without measuring the toxicant substrate concentration. The ED-TOC needs practically no tuning, so it is easy to implement and easy to apply to similar problems.

In Section 2 the particular problem will be stated. The proposed ED-TOC strategy to solve it will be described in Section 3, including basic practical implementation remarks. Section 4 presents the experimental validation in a laboratory setup. Some conclusions close the paper.

2. PROBLEM FORMULATION

The difficulties for treating toxicants in SBRs are easily explained using a non linear inhibitory model. Fig. 1 shows such type of biomass specific growth rates. It is also directly related to the reaction's rate because the biomass grows on substrate. Note that if the toxicant substrate concentration $\boldsymbol{S}$ is maintained near $\boldsymbol{S}$* then the reaction is quick and safe i.e. stays away from the killing zone. If below $\boldsymbol{S}$*, safe but slow. If over $\boldsymbol{S}$*, then it gets slow as the biomass gets inhibited. If $\boldsymbol{S}$ is accidentally pushed much further up, the SBR may even get disabled.

A reaction model for the SBR is given in (1):

$$
\begin{aligned}
\dot{X} &= (m - K_d)X - X\,\frac{Q_{in}}{V} \\
\dot{S} &= -\frac{1}{Y_{X/S}}\,mX + (S_{in} - S)\frac{Q_{in}}{V} \qquad (1) \\
\dot{O} &= -\frac{1}{Y_{X/O}}\,mX - bX + K_l a * (O_s - O) + (O_{in} - O)\frac{Q_{in}}{V} \\
\dot{V} &= Q_{in}
\end{aligned}
$$

Where:

- $\boldsymbol{X}$: Biomass concentration inside the bioreactor
- $\boldsymbol{S}$: Substrate concentration inside the reactor
- $\boldsymbol{O}$: DO concentration
- $\boldsymbol{V}$: Water volume level of the reactor
- $Y_{X/S}$: Biomass/Substrate yield coefficient
- $K_l a$: Oxygen mass transportation coefficient
- K_d: Specific decay biomass rate
- S_{in}: Influent's substrate concentration
- Q_{in}: Influent flow to the reactor
- $Y_{X/O}$: Biomass/Oxygen yield coefficient
- b: Specific endogenous respiration rate
- m: Specific biomass growth rate (see Fig. 1.)
- O_{in}: Influent's DO
- O_s: DO's saturation value

The typical SBR *batch* operation mode does not take any advantage of this model. It just fills the SBR from its residual volume level $\boldsymbol{V_o}$ until full at $\boldsymbol{V_f}$ using the maximum pump capacity. Hence $\boldsymbol{S}$ is quickly raised (Fig. 2a) to some unknown $\boldsymbol{S_{Batch}}$ into the inhibition zone, and hopefully not close to the killing zone (Fig. 1). That is why the biomass starts processing the substrate slowly. The timing is usually tuned-up by an expert and the operation goes in open-loop, so there is no need for costly nor delicate instrumentation. But if the SBR gets too inhibited, a yet polluted effluent will be drawn because the reaction will not have time enough to complete. The operator has no way to know it. Usually then the expert sets the reaction time much larger than needed in order to prevent for this type of disturbances (i.e. influent's concentration peaks). On the other hand, if the reaction's time is set too long, the biomass will starve, as it will have to wait excessively for the next *batch* to feed on. Starvation is another potential problem if it produces deacclimation of the SBR. This is why such fixed time *batch* mode, although easy and apparently economical to operate, provides neither optimization nor robustness for the process.

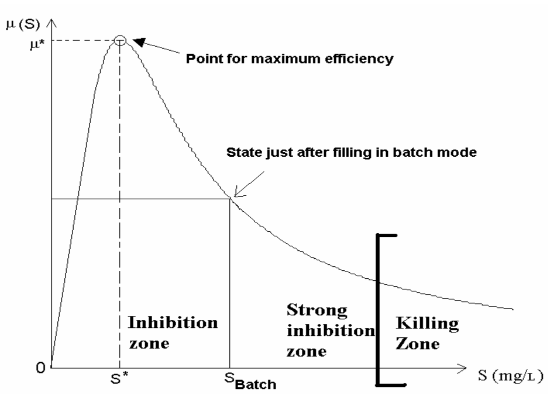

Fig. 1. Inhibitory type Biomass specific growth rate

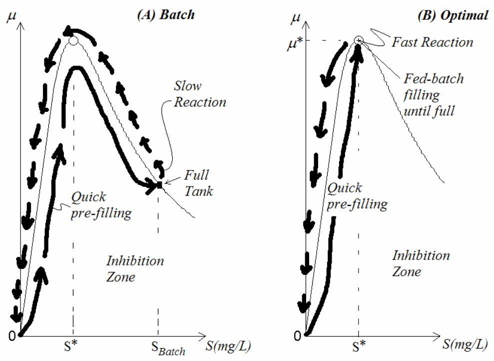

Fig. 2. $\boldsymbol{S}$ Trajectories for: (a) *Batch*, (b) *TOC*

The TOC strategy instead provides for optimality. It uses a *fed-batch* operation mode. That is, to fill the SBR at a controlled rate, not all at once. This combines the filling and reaction stages. Fig. 3 shows its trajectories in the Volume-Substrate plane ($\boldsymbol{VS}$). The control starts the filling as quickly as possible (see also long fat arrow in Fig. 2b), but once $\boldsymbol{S}$* is reached, then it slows down the filling to an inflow rate $\boldsymbol{Q_{opt}}$ that provides just the exact amount of substrate needed to replace the degraded one. That is, it takes the system to its optimal operational point, where the influent replaces continuously the substrate degraded by the biomass (see fed-batch point in Fig. 2b and fed-batch trajectory in Fig. 3). The optimality results from staying at $\boldsymbol{S}$ =$\boldsymbol{S}$* until the reactor gets full (Moreno, 1999). Typically the initial substrate concentration $\boldsymbol{S_o}$ is zero, but two other cases may arise. If 0<$\boldsymbol{S_o}$<$\boldsymbol{S}$* the process will be almost the same as explained before (Fig. 3a). But if $\boldsymbol{S_o}$ is higher than $\boldsymbol{S}$*, then the filling should not proceed until the SBR naturally degrades the substrate down to the critical

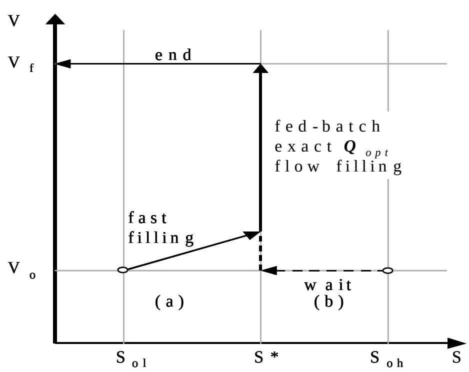

Fig. 3. Optimal mode $\boldsymbol{VS}$ trajectory.
a) $\boldsymbol{S_o}$=$\boldsymbol{S_{ol}}$<$\boldsymbol{S}$*; b) dotted for $\boldsymbol{S_o}$=$\boldsymbol{S_{oh}}$>$\boldsymbol{S}$*

S* value (see dotted trajectory in Fig. 3b). To solve the substrate sensor lack issue, the TOC estimates its concentration by using DO based observers. The main problem with such an approach is that the SBR model (1), that links the DO to the substrate concentration, is full of parameters that are either difficult to measure or uncertain (Schoeb *et al*., 2003). Besides, it needs ***S**** to be precisely known. This renders that type of solution fragile, non robust, and difficult to apply at an industrial level.

The new ED-TOC solves all these problems: It uses only DO measurements that are easy and robust to obtain; it is very robust against model and parameter uncertainties; it achieves robust (almost) time optimality, despite of uncertainties; and it can be made adaptable to increase its performance. This makes it usable at an industrial level. This ED-TOC strategy will be described and the results of its experimental verification will be presented.

3. PROPOSED ED-TOC STRATEGY

Fig. 4 shows the proposed ED-TOC control layout. There is neither the need to know the actual SBR reaction's rate nor the actual substrate concentration. Instead it is necessary to know certain events related to the reaction's rate. A software module estimates a g variable (related to m) used to detect such events. Then an event detector informs the controller the events ***e*** (see Table 1), and the control then chooses the appropriate state s (see Table 2) for the system. Fig. 5 shows the state transitions for the control when specific events ***e*** are detected. It summarizes Tables 1 and 2.

A way to estimate g will be derived next. In the case of interest, the total biomass ***B*** growth for one reaction may be neglected. That is equivalent to say that its kinetics is so slow that it can be assumed constant. Then multiplying eq.<u>1***O***</u> by ***V***, assuming that the inflow has no aeration ($O_{in} \approx 0$), using ***B=XV*** and rearranging the expression, it follows that:

$$g \stackrel{\Delta}{=} \frac{B}{Y_{X/O}} m + bB = K_l a * (O_s - O) * V - OQ_{in} + \dot{O}V \qquad (2)$$

All the variables in the right side of eq. 2 are measurable or straightforwardly computable. The only parameters that need to be known from the model are $K_l a$ and O_s. Both are easy to obtain. The DO needs to be filtered and derived, but as it is a slow-varying signal no practical problems arise from that. The shift phase or time delay introduced by filtering may be countered by introducing a t_s stabilizing time for the signal processing modules.

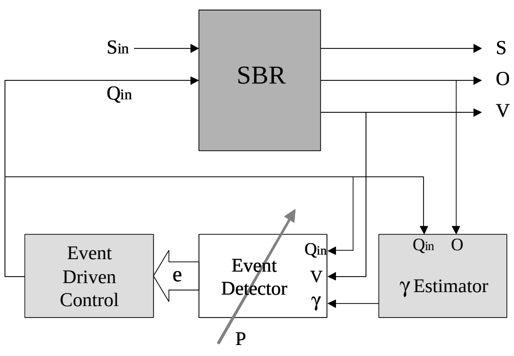

Fig. 4. ED-TOC scheme

The computable g variable as defined in (2) is related to the reaction's rate m by unknown constant parameters. A translation by an unknown ***bB*** constant exists but, except that, it is proportional to m. Compare Fig. 1 and Fig. 6.

Now let's define (see Figs. 5 and 6):

- σ_n finite controller's state tag; n∈[0,N]=(0,1,2,3,4)
- i finite state transitions counter; i∈[0,I]; i=0 at t_0.
- σ^i state after ith transition (i.e. $\sigma^0=\sigma_0$; $\sigma^I=\sigma_N$)
- t_i recorded time for ith transition occurrence.
- $g^* = g(S^*)$, Unknown, non Computable and might Vary slowly over time (UnCV).
- $g_i^* = \max(g^*(t))$ for $t \in [t_i, t_{i+1}]$, real time searchable.
- P tuneable percentage for rate event calculations.
- $g_p = (P/100) g_i^*$, a P percentage of the actual maximum
- S_{pl} substrate concentration at which the reaction rate will be a P percentage of its maximum but S will yet be lower than S^*. UnCV.
- S_{ph} substrate concentration at which the reaction rate will be a P percentage of its maximum, but inside the inhibition zone. UnCV.
- $S_{gap} = S_{ph} - S_{pl}$ substrate concentration space in which the *fill-wait* control cycle evolves. UnCV.
- S_f substrate concentration at which the reaction will be considered to have ended. UnCV.
- $g_f = g(S_f)$, chosen reaction's final stopping threshold.
- t_s Stabilizing time for real time implementation. Choose just big enough to guarantee correct filters/actuator/sensor response to state changes.

<u>Table 1. Robustly Detectable Events</u>

Tag	Meaning	Trigger
e_0	$S < S^*$	$(Q_{in}>0)\&(dg/dt>0)\&(t ³ t_i+t_s)$
e_1	$S ³ S_{ph}$	$(Q_{in}>0)\&(g < g_p)\&(t ³ t_i+t_s)$
e_2	$S £ S_{pl}$	$(Q_{in}=0)\&(g < g_p)\&(t ³ t_i+t_s)$
e_3	$V ³ V_f$	$(V ³ V_f)$
e_4	$S £ S_f$	$(Q_{in}=0)\&(g < g_f)\&(t ³ t_i+t_s)$
e_5	$S > S^*$	$(Q_{in}>0)\&(dg/dt<0)\&(t ³ t_i+t_s)$

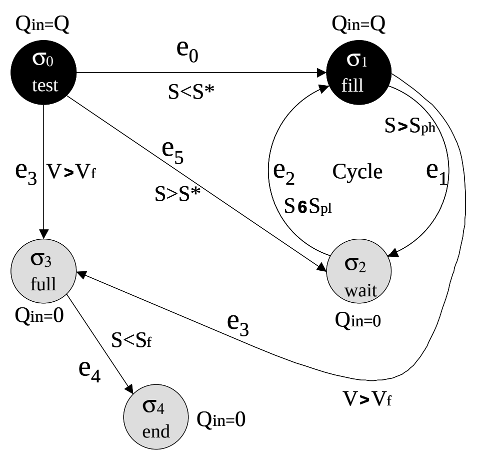

Fig. 5. ED-TOC's finite state transition diagram

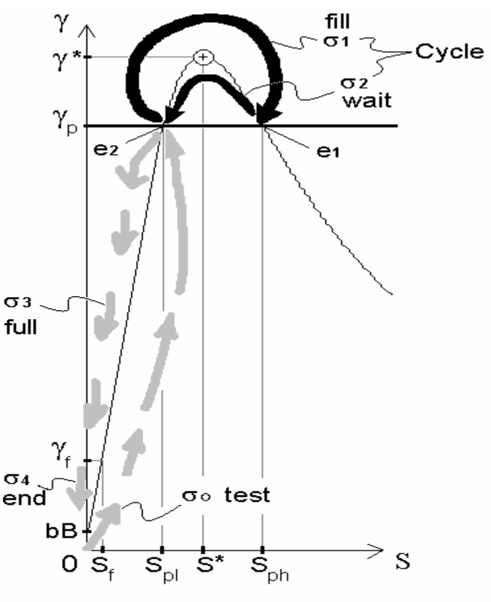

Fig. 6. ***S*** Trajectory for $\boldsymbol{S_o}$=0 (ED-TOC mode)

Table 2. Finite States for the ED-TOC

Tag	Meaning	Action	Exit on/to
σ_0	test	Qin=Q (on)	$\boldsymbol{e_0}\sigma_1, \boldsymbol{e_3}\sigma_3, \boldsymbol{e_5}\sigma_2$
σ_1	fill	Qin=Q (on)	$\boldsymbol{e_1}\sigma_2, \boldsymbol{e_3}\sigma_3$
σ_2	wait	Qin=0 (off)	$\boldsymbol{e_2}\sigma_1$
σ_3	full	Qin=0 (off)	$\boldsymbol{e_4}\sigma 4$
σ_4	end	Qin=0 (off)	settling stage

3.1 ED-TOC operation mode.

A constrain must be established for the ED-TOC to operate properly. It is necessary to guarantee that if influent is applied, then ***S*** will grow. This means that the ***S*** derivative in eq.1***S*** should be made positive. It poses not a hard restriction as it is normally the case. In fact, it allows $\boldsymbol{Q_{in}}$ and $\boldsymbol{S_{in}}$ to vary in any possible way as long as the resulting restraining inequality (3) is satisfied:

$$(S_{in} - S)Q_{in} > \frac{mB}{Y_{X/S}} \qquad (3)$$

If this conditions fails, no harm will come to the SBR. But then no sub-optimality will be guaranteed either.

Note also that if no influent is applied, the substrate ***S*** will tend to zero and *g* will tend to ***bB***. This is because the biomass will consume ***S***.

To explain the ED-TOC operation let's take a look at Figs. 5 and 6. Assume the typical initial conditions $\boldsymbol{S_o}$=0, ***V***=$\boldsymbol{V_o}$, ***i***=0. The initial controller's σ_0 *test* state will turn the influent pump *on*, and a $\boldsymbol{Q_{in}}$=***Q*** satisfying (3) will be applied. Then ***S*** will grow and so will *g* (see ascending grey arrows in Fig. 6). After a $\boldsymbol{t_s}$ time elapses, an event $\boldsymbol{e_0}$ will be detected as proper conditions on Table 1 are met. Then ***i*** increases to ***i***=1 as this is the first state transition. The next state will be the *fill* state σ_1 as defined in Table 2. Such state keeps the inflow running and the search for a maximum g_1* begins for this particular state. The substrate concentration ***S*** keeps raising until it eventually gets to the unknown ***S**** value, and then keeps raising. At this point, some g_1* local maximum is supposed to be registered in the event-detector. Using this value a g_p is calculated. Once the substrate matches up ***S***=$\boldsymbol{S_{ph}}$ then $g = g_p$. Here an event $\boldsymbol{e_1}$ will be detected as proper conditions on Table 1 are met. Then ***i*** increases to ***i***=2 as this is the second state transition. The next state will incidentally be the *wait* state σ_2 as defined in Table 2 (see black little arrow in Fig. 6). Such state stops the inflow by shutting *off* the pump. A new search for a g_2* begins. Meanwhile ***S*** will decrease as the biomass consumes it. Once the substrate matches down ***S***=$\boldsymbol{S_{pl}}$ then $g = g_p$. Here an event $\boldsymbol{e_2}$ will be detected as proper conditions on Table 1 are met. Then ***i*** increases to ***i***=3 as this is the third state transition. The next state will be the *fill* state σ_1 again, and a control cycle will establish (see big black arrow in Fig. 6). The cycle will continue and ***i*** will increase as necessary to fill the SBR tank. Once this happens, the event detector will switch the state to the *full* state σ_3 (see descending grey arrows in Fig. 6). At this point the inflow will cease, and the system will wait for the substrate to be consumed to the $\boldsymbol{S_f}$ value, where $g = g_f$. Then an event $\boldsymbol{e_4}$ will be detected as proper conditions on Table 1 are met. This means that the reaction is considered practically finished. The system will then rest at the *end* state $\sigma^I = \sigma_N = \sigma_4$ until an outer control loop takes the system to the settling stage, usually after waiting some short extra safety time to guarantee substrate depletion.

More general initial condition cases will be explained using the ***VS*** trajectories. In Fig. 7a the case for 0<$\boldsymbol{S_o}$<***S**** is shown, which behaves much the same as the one explained before. The abnormal case for initial condition where $\boldsymbol{S_o}$>***S**** is shown in Fig. 7b. There the difference is that the σ_0 *test* state will allow the controller to detect that the system is inside the inhibition zone. So it will first switch to the σ_2 *wait* state instead of going right into the σ_1 *fill* state.

3.2 Sub-optimality

By using Fig.7 it is easy to shown that, under proper limit case assumptions, the ED-TOC will approach the TOC controller's behaviour shown in Fig.3. If instrumentation and practical real time derivatives could be thought as instantaneous, then $\boldsymbol{t_s}$ could be set to zero, or at least approach to it. In such case the σ_0 *test* state will occupy only an instant in time. Then the σ_0 arrows in Fig. 7 will almost disappear into a single point. Now, by looking at Fig. 6, it can be seen that if ***P***→100% then $g_p \to g$* and so both $\boldsymbol{S_{pl}}, \boldsymbol{S_{ph}} \to$ ***S****. This means that $\boldsymbol{S_{gap}}$ will be reduced to almost zero width in Fig. 7a, forcing the zigzagging rising trajectory to approach a vertical line. It also means that the total number of state transitions ***I*** will increase, and in fact ***I***→∞.
It follows that $\boldsymbol{Q_{in}}$ will be a heavily chopped signal with an instantaneous mean value approaching $\boldsymbol{Q_{opt}}$ (Moreno, 1999). This means that the ED-TOC

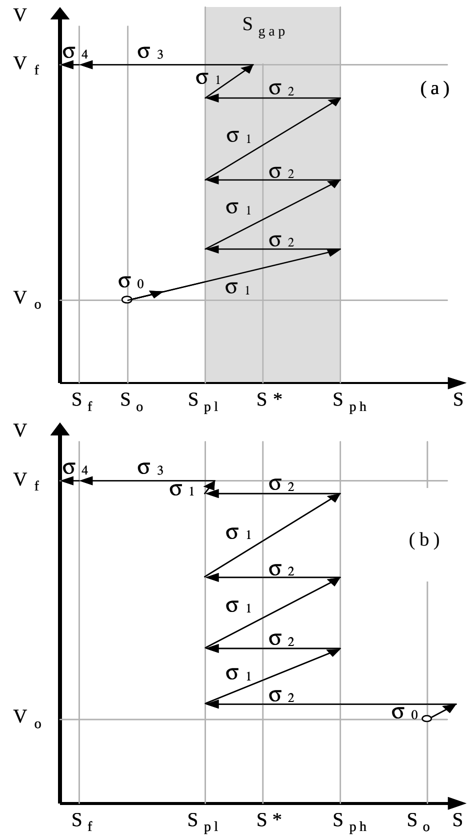

Fig. 7. ***VS*** Trajectories for a) $S_o<S^*$; b) $S_o>S^*$

approaches the optimal mode of operation when $\boldsymbol{P}\rightarrow 100$ and $\boldsymbol{t_s}\rightarrow 0$

3.3 Remarks on Robustness

The ED-TOC does not need to know the model of neither the SBR nor the biomass growth i.e. it will work and keep its properties for any inhibitory model and even for a model as different as the non inhibitory Monod type. So it is independent of changes that may occur in this models, whether or not those changes happen during a single reaction or in a long term basis. The two used parameters $\boldsymbol{K_l a}$ and $\boldsymbol{O_s}$ are easy to find experimentally and are unlikely to change in the short term.

3.4 Adaptability

It is interesting to note that some information about the quality of $\boldsymbol{Q_{in}}=\boldsymbol{Q}$ can be gathered from timing the σ_1 *fill* state. This can be used to control and adapt the influent flow. In fact, if $\boldsymbol{Q}=\boldsymbol{Q_{opt}}$, then the system will stay in the *fill* state and no state transitions will happen while filling (but not the other way around). On the other hand, if $\boldsymbol{Q}>>\boldsymbol{Q_{opt}}$, then some heavy state switching will occur. So it is possible to set a desired switching rate, and then adapt $\boldsymbol{Q_{in}}$ value to track it. Then a switching time $\boldsymbol{T_{sw}}$ must be chosen, bigger than the instrumentation's and SBR's response times, for the adaptive system to behave appropriately.

Let $\boldsymbol{j}$ be some state transition for which $\sigma^j=\sigma_1$. Then $\boldsymbol{T_j}=\boldsymbol{t_{j+1}} - \boldsymbol{t_j}$ will be the time spent in that particular σ^j *fill* state. Let's define $\boldsymbol{Q^j}$ as the mean value during σ^j for a sufficiently smooth $\boldsymbol{Q}$. Once the system leaves such σ^j state, a desired $\boldsymbol{Q_{des}}^{j+2}$ may be calculated for the next $\boldsymbol{t_{j+2}}$ time the system may enter the σ_1 *fill* state. If $\boldsymbol{T_j}>\boldsymbol{T_{sw}}$ this means $\boldsymbol{Q^j}$ was less than its desired -but unknown- value. Similarly $\boldsymbol{T_j}<\boldsymbol{T_{sw}}$ means $\boldsymbol{Q^j}$ was higher than such desired value. Then the proposed adaptive law for $\boldsymbol{Q}$'s mean value is presented in (4)

$$Q_{des}^{j+2} = Q^{j}\,\frac{T_j}{T_{SW}} \qquad (4)$$

4. EXPERIMENTAL RESULTS

The ED-TOC strategy was proven experimentally using a $\boldsymbol{V_f}$ =7L SBR inoculated with sludge biomass from a municipal WW treatment plant (WWTP), with $\boldsymbol{X_0}$=2500mg/L for a residual volume $\boldsymbol{V_0}$=3L. The toxicant synthetic substrate was 4-chloro-phenol (4CP) dissolved in water with appropriate nutrients (Buitrón *et al.*, 2003). A software was developed in which $\boldsymbol{T_{sw}}$=0.25h and $\boldsymbol{P}$=88% were used. A DO sensor for the reactor's water and a flow controllable peristaltic pump for the influent were attached to the computer, with the use of the appropriate I/O hardware.

A series of experiments were done and compared to the standard *batch* mode of operation. The long term treating of a concentration of only more than 700 mg/L of 4CP would jeopardize the operability of the SBR in the standard *batch* mode (Buitrón *et al.*, 2003). Thus in the standard conditions the substrate concentration used was S_{in}=350 mg/L 4CP.

Experiments using the ED-TOC strategy applied the same 350 mg/L of 4CP first, then doubling it every other reaction. Fig. 8 shows an experiment for 5600mg/L of 4CP. Concentrations up to 11200mg/L were treated. It is very unlikely to find such huge concentrations even in the worst industrial cases. This kind of concentration would have killed the *batch* operated SBR almost instantly. Instead, the overall efficiency of the ED-TOC operated SBR improves even further at high concentrations, as the total substrate (toxicant) mass gets treated in a single cycle.

To treat a given high concentration in *batch* mode, the substrate would have to be pre-dissolved in additional water, to match down the standard 350mg/L concentration. Thus, more *batches* would be needed, each one spending additional time in non productive stages as settling, drawing, and idling. This means that the efficiency of the new ED-TOC system compared to the standard *batch* mode, as a whole, increases even more when exposed to peak concentrations. To degrade 22.4g of 4CP a total of 16*batches**3.5h/*batch*=56h are needed. Using ED-TOC instead only one cycle is needed for doing the same. It lasts 21h (Fig. 8) including settling and drawing stages. This yields a 62% overall time improvement.

Fig. 8a shows the DO kinetics for the whole 5600mg/L of 4CP reaction. Samples of substrate

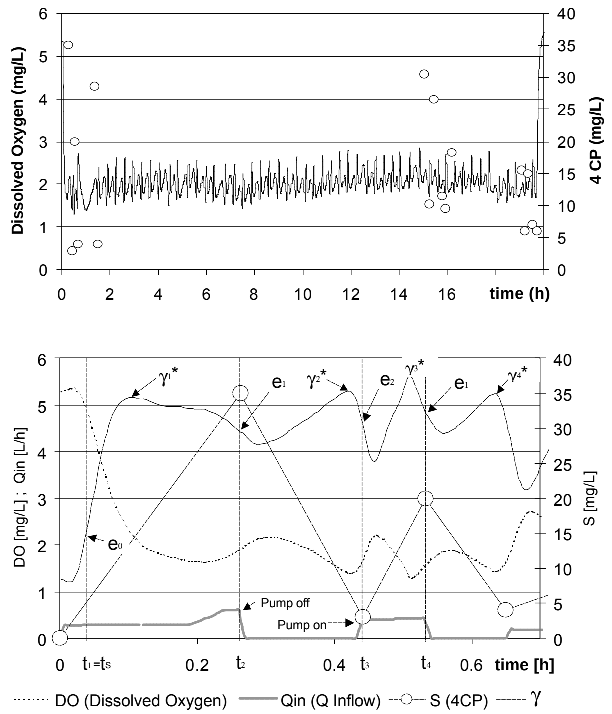

Fig. 8. a) ED-TOC experiment for S_{in}=5600mg/L of 4CP
b) Zoom detail of the first two *fill-wait* cycles

concentration were taken at the marked time points and analysed off-line using colorimetric techniques.

Fig. 8b shows a detail of the same reaction, a fraction of the first hour. There the controller's dynamics can be seen. Once the influent begins to be pumped into the reactor the reaction starts. The DO decreases as the biomass increases its metabolic consumption to degrade the 4CP. Simultaneously, the estimator calculates g and follows its value. At the maximum point, between $\boldsymbol{t_1}$ and $\boldsymbol{t_2}$, a local g_1* is detected and stored. Note that such maximum appears prior to the oxygen minimum. The detected maximum is later used to compute the g_p threshold and then detect the $\boldsymbol{e_1}$ event that appears later at $\boldsymbol{t_2}$. At such time the influent pump is turned off. A sample of substrate reveals that the concentration is as low as expected. After some time, the natural reaction dynamics consumes the substrate and then an $\boldsymbol{e_2}$ event is detected at $\boldsymbol{t_3}$. A new substrate sample is taken and again its value is as expected. At this point the pump is started again and the control cycle begins.

As the proposed method relies heavily on the value of $\boldsymbol{K_l}a$, a series of simulations to test its sensitivity were made. The system kept working even when misestimating $\boldsymbol{K_l}a$ in the (-30%,+100%) error range.

6. CONCLUSIONS

An *Event-Driven Time Optimal Control* (ED-TOC) scheme for Sequencing Batch Reactors (SBR) was successfully designed and tested. The advantages over the previously known controllers are multiple. There is neither the need to know the influent's toxic substrate concentration to be treated nor the one inside the SBR. Instead a dissolved oxygen (DO) sensor in the SBR tank is used for closing the control loop. The DO sensors are widely available, robust and economical. Therefore the ED-TOC is practically realizable, robust and (almost) optimal.

The use of this controller in a SBR WWTP will increase its speed, allowing to reduce the plant's size. Even more, it allows for a safe treatment of influents with unknown high concentration peaks of toxicants. It is safe for the plant and safe for the environment.

The basis for an adaptive inflow strategy are set. More work needs to be done on the subject, to formalize the properties of the ED-TOC, and also to characterize the whole class of systems in which it might be useful.

ACKNOWLEDGEMENTS

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PRACTICAL OPTIMAL CONTROL FOR FED-BATCH BIOREACTORS

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Abstract: Optimal operation of fed-batch bioreactors is an important practical issue. Since control actions are saturation-limited, the optimal control consists usually of both singular and bang-bang arcs. However, its realization requires good model knowledge and also measurement of all state variables, requirements hardly satisfied in real applications. In this paper a method is proposed, for a class of bioreactors, to robustly optimize the operation when few measurements are available and the model is uncertain. Such control law is justified and its properties analyzed. The class of processes addressed includes a biomass growth bioreactor and an experimental wastewater treatment plant for degrading toxicants.

Keywords: optimal control, software sensor, robust control, control applications, fed-batch bioreactor.

1. INTRODUCTION

Many important industrial fermentation processes, for the production of antibiotics and enzymes or for the treatment of wastewater, are carried out using bio-reactors operated in fed-batch mode. Since it is reasonable to improve their performance, optimal control theory has been used to determine the best control policy (Smets et al., 2002; Sarkar and Modak, 2003; Moreno, 1999). Such strategy can be described as a feedback control law, and it is usually necessary to know perfectly the model of the plant, and to measure the whole state to implement it. In many applications these two conditions are very restrictive: a perfect model and parameter knowledge is very often unrealistic, and in biotechnology and wastewater treatment it is either impossible or very expensive to measure all state variables. In order to cope with the first problem different robust approaches have been proposed in the literature. Most often different adaptive algorithms identify the parameters of the (otherwise assumed well known) mathematical model, and adapt accordingly the control strategy (Bastin and Dochain, 1990; Van Impe and Bastin, 1995; Van Impe, 1998). Adaptive Extremum-Seeking strategies have been also proposed (Marcos *et al.*, 2004; Titica *et al.*, 2003). Although the methodology is most appropriate for continuous reactors, where an optimal steady state operation is searched, under suitable conditions it can also operate correctly for fed-batch processes (Betancur *et al.*, 2004b).

In this work a different approach to deal with the lack of measurements and the uncertainty in the model, while optimizing operation, of a class of bio-reactors will be proposed. The main idea is based on the following observations. Usually, the exact optimal control, when the realistic assumption of limited input variables is done, can be decomposed in bang-bang and singular arcs. When this solution can be implemented via feedback the information required for the bang-bang part is very low, and its implementation is very robust to model uncertainties. More problematic is the determination and implementation of the singular arc. It requires basically a good knowledge of the model and parameters of the plant, and it is usually very sensitive to uncertainties. Our method proposes to replace the sensitive and smooth singular control by a bang-bang one that maintains the system trajectory around the singular surface. The produced error can (theoretically) be made as small as desired (Hermes and LaSalle, 1969; Moreno, 1999). The advantage of this replacement is that it is usually very robust against uncertainties and, for its implantation, a reduced quantity of information is required (Moreno, 1999). The robustness of this implementation is linked to the well-known properties of Sliding Mode Control (Khalil, 2002; Slotine and Li, 1991). The requirement of low quantity of information is related to the fact that it is only necessary to determine the singular surface in the state space. This surface is usually associated to some events on internal variables. If such events could be software-sensed using just the measurable variables, then a practical solution is feasible. Moreover, if the switching or singular surfaces are robustly related to these variables, the approach can be made robust against model changes or uncertainties.

In the following section the class of problems for which these ideas are developed will be introduced. In Section 3 the previously outlined strategy will be carried out for these problems. In Section 4 some experimental results will be presented.

2. PROBLEM FORMULATION

The optimization problem for a class of simple microbial growth process in a fed-batch bioreactor is considered, using the following dynamical model (Smets et al., 2002):

$$\frac{dX}{dt} = \mu X - \frac{F}{V}X \tag{1}$$

$$\frac{dS}{dt} = -(k_1\mu + m)X + \frac{F}{V}(S_i - S) \tag{2}$$

$$\frac{dV}{dt} = F \tag{3}$$

where states X *(g/L)* and S *(g/L)* hold for biomass and substrate concentrations, respectively, μ *(h^{-1})* is the specific growth rate, S_i *(g/L)* denotes the concentration of the substrate in the inflow, k_1 is a yield coefficient, m is a maintenance constant, F *(L)*, the control variable, is the inflow and V *(L)* is the volume of the liquid medium in the tank. $\mathbf{z}^{\mathrm{T}}=[X, S, V]$ represents the state vector, that is restricted to the set

$$\Omega = \left\{ \mathbf{z} \in \Re^3 \ \middle|\ 0 < X; 0 \le S \le S_{\max}; 0 < V_o \le V \le V_{\max} \right\}. \tag{4}$$

The input is restricted to $0 = F_{\min} \le F \le F_{\max}$. For any system variable ϕ let's denote its value at instant t as $\phi\,(t,t_0,\mathbf{z}_0,F)$ for input F, being $\mathbf{z}_0$ the state at $t_o < t$.

Inhibitory specific growth rates will be considered, although everything is also valid for μ monotonic. They are described by a non-monotonic function of the substrate concentration, like the Haldane law:

$$\mu(S) = \frac{\mu_0 S}{K_S + S + S^2 / K_I} \tag{5}$$

where μ_0 is a parameter related to the maximum value of the specific growth rate μ^*, K_S denotes the saturation and K_I the inhibition constant. In general, it will be assumed that $\mu(S)$ grows monotonically for $S\in[0,S^*]$ and decreases for $S\in[S^*,\infty]$. Such a model is typically used to describe the substrate inhibition effect in fed-batch bioreactors, as shown in Figure 1.

In industrial fermentations (e.g. production of baker's yeast) the aim is to maximize the total biomass at the end of the process (Smets et al., 2002), but when $m>0$ this amounts to minimize the reaction time. For Waste Water Treatment Plants (WWTP) m is usually considered to be zero and the objective is to minimize the time necessary to degrade the substrate (Moreno, 1999). The measured variables depend strongly on the application. In general, it is difficult and expensive to measure biomass and substrate concentrations, but it is easy to measure volume, gaseous products and dissolved oxygen concentrations. For the biotechnological application it will be assumed that the gas production $y = k_2\mu X$ is measurable, and then, using the volume V, it is possible to calculate y_B, which will be used for the control implementation:

$$y_B = yV = k_2\mu XV = k_2\mu B \tag{6}$$

where $B = XV$ *(g)* is the total Biomass.

For the WWTP it is assumed that Dissolved Oxygen concentration O *(g/L)* and volume level V *(L)* are measured. Using its dynamics

$$\frac{dO}{dt} = -(k_3\mu + b)X + K_l a(O_s - O) - \frac{F}{V}O \tag{7}$$

and (2), the variable y_W can be calculated:

$$y_W = (k_3\mu + b)B = K_l aV(O_s - O) - FO + V\frac{dO}{dt} \tag{8}$$

For the WWTP the variable S_i is a (possibly) time-varying perturbation term difficult to measure, but it is a known constant for the biotechnological process. For both systems the functional description of the specific growth is not well known so (5) is only an approximation. The objective is to design an optimal control law that uses the measured variables, respectively y_B and y_W, and that is robust against uncertain model and uncertain parameters.

3. CONTROL STRATEGY

The design of a control law that satisfies the imposed requirements will be explained in three steps.

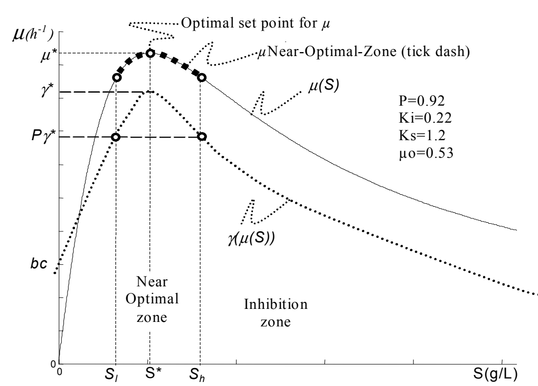

Figure 1. Haldane's type biomass specific growth rate. The dotted line depicts a measurable $\gamma=(a\mu+b)c$

3.1. Exact optimal control law

For both systems the optimal control law for one batch consists of two bang-bang arcs, and an intermediate singular arc. The batch finishes when $V=V_{max}$ and $S \leq S_{end}$, where S_{end} is some (small) rest substrate value. The optimal control law, to minimize reaction time, is given by (Smets et al., 2002; Moreno, 1999)

$$F_{opt} = \begin{cases} 0 & if \quad V = V_{\max} \; or \; S > S^* \\ F_{\sin} & if \qquad S = S^* \\ F_{\max} & if \qquad S < S^* \end{cases} \tag{9}$$

where
$$F_{\sin} = \frac{k_1(\mu + m)VX}{S_i - S} \tag{10}$$

is the control inflow along the singular arc, and S^* is the value where μ reaches its maximum μ^*. Define the function $T(F,\mathbf{z}_0)$ to represent the time necessary to bring the initial state $\mathbf{z}_0$ to the target set $Z_f=\{(X,S,V)/ S \leq S_{min} \wedge V \geq V_{max}\}$ using F as input (the other model parameters are fixed). $T_{opt}(\mathbf{z}_0)=T(F_{opt}, \mathbf{z}_0)$ corresponds to the optimal path. Note that in the state space Ω the surfaces defined by $S=S^*$ and $V=V_{max}$ are, respectively, the singular and a switching surface. Note that implementation of feedback law (9) requires, in principle, good knowledge of the model of the plant and the measurement of all state variables.

3.2. Approximated optimal control law

A well-known result (Hermes and LaSalle, 1969) states that any trajectory of a nonlinear system can be arbitrarily well approximated by one generated using a bang-bang control law. So, it is possible to approximate the time optimal trajectory generated by the control law (9) with a bang-bang one. This corresponds in this case to the approximation of the trajectory along the singular arc with a bang-bang one (Moreno, 1999). Since the performance criterion does not depend on the input function, and it is continuous with respect to the trajectories, then the optimal index is arbitrarily nearly reached by the approximated trajectory. For the problem at hand this has also been directly demonstrated by (Moreno, 1999).

Approximate control laws can be generated in different forms. They differ basically in the information required to implement them. Some examples will be discussed in the following paragraphs. The following assumption will be made:

Assumption 1: In the state space Ω it is satisfied that

$$\frac{dS}{dt} = -(k_1\mu + m)X + \frac{F_{\max}}{V}(S_i - S) > \varepsilon > 0 \tag{11}$$

Note that inequality (11) has to be satisfied for $S \leq S^*$ for the control law (9) to be feasible, and so it is a natural condition for the problem.

3.2.1. Suboptimal control law using S

If S is measured and S^* is known, then selecting values $0 < S_l < S^* < S_h$ (see Figure 1) the following control law approximates arbitrarily well the optimal trajectory (Moreno, 1999)

$$F = \begin{cases} 0 & if \quad V = V_{\max} \; or \; S \geq S_h \\ F_{\max} & if \qquad S \leq S_l \end{cases} \tag{12}$$

In the interval $S_l < S < S_h$ the control function can, in fact, take any value but, in order to obtain a bang-bang cycle, the previous one is kept until the other extreme is reached (this is a hysteresis effect, see Figure 2). Moreover, when $S \leq S_{end}$ and $V \geq V_{max}$ then the reaction phase is finished and a new cycle may be started.

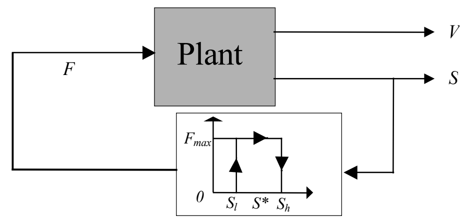

Figure 2. Control scheme for S measurable, S^* known. Control of Volume not shown for simplicity

The important feature of this control law is that, since

$$\frac{dS}{dt} = -(k_1\mu + m)X < 0 \,, \forall \mathbf{z} \in \Omega / \{S = 0\} \tag{13}$$

and because of Assumption 1, every system trajectory tends to the set $S_l \leq S \leq S_h$, stays there until the reactor is full, and then reaches the final set Z_f, finishing the reaction phase. Moreover, if Assumption 1 is satisfied, substrate $S(t,t_o,S_l,F_{max})$ increases monotonically until it reaches S_h, and $S(t,t_o,S_h,0)$ decreases monotonically until S_l. It is important to note that the trajectory is confined to the set $S_l \leq S \leq S_h$, independently of and without knowledge of the parameters and/or the exact form of the growth rate and of the value of the input substrate concentration S_i.

Theorem 1:(Moreno,1999) Suppose that system (1-3) is given, S is measured and S^* is known. Then replacing the optimal control law (9) by the approximate control law (12) the time to reach the target, from any initial condition $\mathbf{z}_0 \in \Omega$, is $T(F,\mathbf{z}_0) = T_{opt}(\mathbf{z}_0)+\Delta(F, S_l, S_h, \mathbf{z}_0)$ with $\Delta(F, S_l, S_h, \mathbf{z}_0)$ continuous and finite and $\Delta \rightarrow 0$ as $S_h, S_l \rightarrow S^*$. i.e. the target will be reached in finite time, and the time along the approximate trajectory can be made as near to the optimal one as desired. This is true for any form of the growth rate (positive if S positive), for unknown S_i and for any positive value of parameters k_1, m.

Note that the approximate control law is robust against model and parameter uncertainties and/or changes. Moreover, it requires little information from the system: only S needs to be measured and S^* and the instant when $V=V_{max}$ need to be known.

3.2.2. Robust Suboptimal control law using f(μ)

If instead of S an appropriate but unknown function of μ is available, i.e. $\gamma=f(\mu)$, then it is possible to derive a control law that approximates arbitrarily well the optimal one. It will be assumed that $f(\mu)$ is a strictly monotonic increasing and continuous function of μ, as for example $f(\mu)=(a\mu+b)c$; for a,b,c unknown constants, $a,c>0$. The maximum $\gamma^* = \max_{S\geq 0} f(\mu(S)) = f(\mu^*)$

is then well defined. It should be noted that it is not necessary to know the exact shape of μ or $f(\mu)$. If Assumption 1 is satisfied, and because the monotone increasing (decreasing) behavior of $S(t)$ when it goes from S_l to S_h (from S_h to S_l, respectively), it is clear that $\gamma(t)$ increases from $\gamma_l = f(\mu(S_l))$ ($\gamma_h = f(\mu(S_h))$) until maximum γ^* and then decreases until γ_h (γ_l respectively). If γ^* is assumed constant but unknown, this leads to scheme in Figure 3. There, an Events Software Sensor (ESS) estimates a maximum of $f(\mu)$ in real time, as $\gamma_\kappa^*(t)=\max(f(\mu(S(\tau))))$ for $\tau\in(t_k,t)$, were t_k is the instant when the last k^{th} state change in the Event Driven Optimal Controller (EDOC) took place.

Comparing the actual values of γ and γ_κ^* allows to determine if $S=S_l$ or $S=S_h$ have been reached, even if S, S_l and S_h remain unknown. In particular, consider $S_l<S^*$ and $S_h>S^*$ such that $f(\mu(S_l))=f(\mu(S_h)) =P\gamma^*$, where $0<P<1$ is a near-optimality control parameter. Making P close to one renders S_l, S_h close to S^*. Figure 1 shows the relation between S_l, S_h, γ^* and P for the case $\gamma = f(\mu) = (a\mu+b)c$. The ESS also determines easily if $S>S^*$ or not, i.e. if the system is in the inhibition zone.

Table 1. ESS events for fed-batch processes

Tag	Trigger	Estimation	Meaning
$e_{1.0}$	$d\gamma/dt>0$	$S<S^*$	Not Inhibited
$e_{2.0}$	$d\gamma/dt<0$	$S>S^*$	Inhibited
$e_{2.1}$	$\gamma\le P\gamma_\kappa^*$	$S=S_h$	MustWait
$e_{1.2}$	$\gamma\le P\gamma_\kappa^*$	$S=S_l$	MustFill
$e_{3.}$	$V\ge V_{max}$	(measured)	TankFull
$e_{4.}$	$\gamma<\gamma_{end}$	$S<S_{end}$	EndReaction

Table 1 shows the events estimated by the ESS. Using such events the EDOC shuts down or powers up the influent pump F as appropriate. The finite state EDOC is depicted in Figure 4. The initial state at $k=0$ for $t=t_0=0$ is always σ_0. If inhibited, the system will jump instantaneously to state σ_2. After the initial bang-bang arc, the cycling between σ_1 and σ_2 will approximate the singular arc. Once the tank is filled, σ_3 will complete the last bang-bang arc. The reaction finishes when σ_4 is reached. After this the rest of the batch sequence (settling, draw…) may be completed and afterwards a whole new cycle may be started. A result similar to Theorem 1 applies in this case.

Theorem 2: Suppose that system (1-3) is given, that a continuous and strictly monotone increasing function $f(\mu)$ of μ is available, and Assumption 1 is satisfied. Assume, furthermore, that γ^* is constant for each batch cycle, but unknown. Then replacing the optimal control law (9) by the EDOC law the time to reach the target from any initial condition $\mathbf{z}\in\Omega$ is

$$T_{EDOC}(F,\mathbf{z}_0)=T_{opt}(\mathbf{z}_0)+\Delta(P,\mathbf{z}_0)+\delta \qquad (14)$$

with $\Delta(P,\mathbf{z_0})$ continuous and finite and $\Delta\to 0$ as $P\to 1$. i.e. the target will be reached in finite time, as near to the optimal one as desired, up to a small value $\delta>0$. This is true for any form of the growth rate (positive if S positive), of the function $f(\mu)$, for unknown S_i and for any values of the parameters $k_1>0$, $m\ge 0$.

Proof (sketch): Similar to the proof of Theorem 16 in (Moreno,1999) and Theorem 3. The important observation here is that limits $P\gamma^*$ given in terms of $f(\mu)$ correspond (in an unknown form) to limits $S_l<S<S_h$ in S (because of the continuity of μ and $f(\mu)$ with respect to S). The value $\delta>0$ is introduced by the initial test (Figure 4) when $S_0>S^*$. Its value depends on the time it takes the ESS to determine the first event. ■

Robustness: Analyzing the event triggers in Table 1 for transitions between σ_1 and σ_2, i.e. $e_{1.2}$ and $e_{2.1}$, it follows that, even if for some reason (i.e. noise or perturbation) the system enters a wrong state, after some time the conditions for a transition to the correct state will always appear. This is so because even if the detected γ_κ^* is not the maximum i.e. γ^*, at some time a $\gamma=P\gamma_\kappa^*$ will be found. Note that the approximate control law is robust against model and parameter uncertainties and changes. Moreover, it requires low information from the system: only $\gamma=f(\mu)$ and the instant when $V=V_{max}$ have to be known, and the finishing value γ_{end} given. It is important to note that the trajectory is confined to set $S_l\le S\le S_h$ independently of and without knowledge of the parameters, the exact form of the growth rate, of $f(\mu)$ and of the value of S_i.

3.3. Robust general near-optimal control law

In the previous paragraph a suboptimal control law was given. If estimations in Table 1 are exact, it can be made as near to optimality as desired by selecting appropriately the parameter P. However, this property depends strongly on the availability of an exact value for γ. If there is some measurement noise or perturbation, if the parameters vary in time or as function of some other state variables, then Theorem 2 is no longer valid as estimations in Table 1 might have errors. In this Section it will be shown that, under reasonable circumstances, the estimation errors are tolerably low and so the approximated control still behaves correctly and robustly. The tradeoff is that optimality cannot be arbitrarily well approximated.

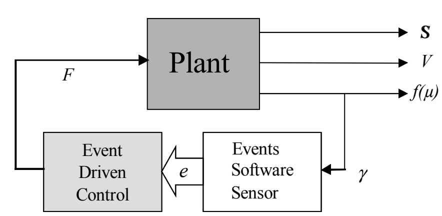

Figure 3. Event Driven Optimal Control scheme

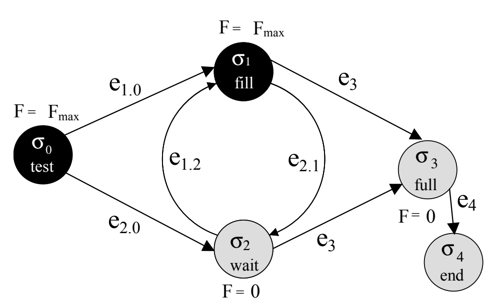

Figure 4. Finite state transitions for EDOC

Note that the practically possible measurements for the two case systems, (6) and (8), are of the form $\eta = f(\mu)B = \gamma B$. Since the total biomass $B=XV$ satisfies $dB/dt = \mu B$, it is clear that it is not a constant but a monotone increasing function of time, and η does not have the required form for the EDOC. Let us analyze its behavior when instead of γ the measured η is used.

Along a trajectory of the plant it is easy to see that

$$\dot{\eta} = (\dot{\gamma} + \mu f(\mu))B = (f'\mu'\dot{S} + \mu f(\mu))B \qquad (15)$$

Where φ' represents the derivative of φ with respect to its argument. When $dS/dt > 0$, which is always satisfied if $F=F_{max}$ under Assumption 1, $sign(d\gamma/dt) = sign(\mu')$. When $dS/dt < 0$, i.e. when $F=0$, $sign(d\gamma/dt) = - sign(\mu')$. Note from (15) that the behavior of η does not reflect that of γ, and the EDOC would work wrongly. However, if $\mu f << f'dS/dt$ one would expect that the behavior of η approximates that of γ, and the EDOC would work correctly.

Theorem 3: Suppose that system (1-3) is given, with continuously differentiable μ. Suppose that $\eta=f(\mu)B$, with B the total biomass and $f(\mu)$ a continuously differentiable and strictly monotone increasing function of μ, is available and Assumption 1 is satisfied. Assume, furthermore, that $\gamma^* = \max f(\mu)$ is constant for each batch cycle, but unknown. Suppose that there exists some $S_{\max} > S_2 > S^*$ such that for $\Omega \cap [S_2, S_{max}]$

$$\left(\left[-(k_1\mu + m)X + \frac{F_{\max}}{V}(S_i - S)\right]f'\mu' + \mu f(\mu)\right) > 0, \qquad (16)$$

and that there exists $0 < S_1 < S^*$ such that for $\Omega \cap (0, S_{max}]$

$$\left(-(k_1\mu + m)Xf'\mu' + \mu f(\mu)\right) < 0. \qquad (17)$$

Denote as $B_{\max}=\max_{\mathbf{z}_0\in\Omega} B(T_{opt},0,\mathbf{z}_0)$ the maximal quantity of biomass that can be obtained in the reactor, and as $B_{\min}$ the minimal possible quantity of biomass in the reactor. It is said that $P \in (0,1)$ is feasible if there exist $0 < S_3 < S_l$ and $S_2 < S_4 < S_{max}$ such that $Pf(\mu(S_1))B_{\min} = f(\mu(S_3))B_{\max}$, $Pf(\mu(S_2))B_{\min} = f(\mu(S_4))B_{\max}$ are satisfied. Suppose that there exists a feasible P_f. Then replacing γ by η in EDOC law, the time to reach the target from any initial condition $\mathbf{z} \in \Omega_I$ and for any $P \in [P_f, 1)$ is

$$T_{ROB}(\mathbf{z}_0) = T_{EDOC}(\mathbf{z}_0) + \Xi(P, \mathbf{z}_0) \qquad (18)$$

with $\Xi(P,\mathbf{z}_0)$ continuous and finite, i.e. the target will be reached in finite time. However, when $P \rightarrow 1$ it is not always true that $\Xi(P,\mathbf{z}_0)$ tends to zero.

Proof: Note that if P_f is feasible, so is every $P \in [P_f, 1)$. From (15) and Assumption (16) it follows that when $\mathbf{z}_0 \in \Omega_I$ is such that $S_0 \notin [S^*, S_2]$ (and EDOC is in σ_0) then $sign(d\gamma/dt)=sign(\mu')$, and the transitions are the same when using η instead of γ. If $S_0 \in [S^*, S_2]$, then both transitions $e_{1.0}$ or $e_{2.0}$ are possible.

Now suppose that the EDOC is in σ_1 and $S \leq S^*$. Then from (15) it follows that $\text{sign}(d\eta/dt)>0$, and $\gamma_k^*(t_k)=\eta(t_k)$. Then γ, η and S increase until $S=S^*$, at $t=t_k+T^*$, where $\gamma_k^*(t)=\eta(t_k+T^*)$. At this point γ begins to decrease, although η can increase further. However, because of (16), η is decreasing at the latest when $S=S_2$. Furthermore, if e_3 is not reached before, the state transition $e_{2.1}$ is satisfied at the latest when $S=S_4$.

Now suppose that the EDOC is in σ_2 and $S \geq S^*$. Then $sign(dS/dt)<0$, $sign(d\eta/dt)<0$, and $\gamma_k^*(t_k)=\eta(t_k)$. Then γ, η increase and S decreases until $S=S^*$, at $t=t_k+T$, where $\gamma_k^*(t)=\eta(t_k+T^*)$. Although at this point γ begins to decrease, η can still increase further. However, because of (17), η is decreasing at the latest when $S=S_l$. Furthermore, if e_3 is not reached before, the state transition $e_{1.2}$ is satisfied at the latest when $S=S_3$.

Note that once σ_1 or σ_2 have been reached, then the substrate S stays in the set $[S_3,S_4]$ until σ_3 is reached. If the EDOC is in σ_1 and $S \in [S^*,S_2]$ it is clear that at the latest when $S=S_4$ the state transition $e_{2.1}$ gets satisfied.

Note that when $P \rightarrow 1$ then $[S_3,S_4] \rightarrow [S_1,S_2]$, but it is not true that $\Xi(P,\mathbf{z}_0)$ tends to zero. ■

Some remarks are in order:

- (16) and (17) are satisfied if, for example, the relative change $|f'\mu'/f\mu|$ is big outside a vicinity of S^*, and if F_{max} and/or S_i are big. Note also that as $(S_2-S_1) \rightarrow 0$ the results of EDOC are recovered.
- For WWTPs the change in B during one cycle is very small, since the amount of toxics that can be treated is typically small compared to B. This means that (16) and (17) are typically satisfied, that S_2-S_1 is very small, and therefore the loss of optimality is small. Successful experimental results are available in (Betancur et al., 2004a). For biotechnology process, instead, the change in B is usually large. Even for such a case simulation results show the effectiveness of the EDOC (Betancur et al., 2004b).
- The form of μ and f influence how big is the minimum loss of optimality.
- No noise analysis has been carried out because of lack of space. However, it can be done in a similar fashion as the proof of Theorem 3.
- In practice, derivatives for Equation (7) and Table 1 are not available. They are calculated using numerical real-time methods. This introduces some time delays and distortion in the derivative signal. The same is true for signals generated using real practical sensors devices. A way to deal with such time delays is given in (Betancur et al., 2004a). Distortions could be treated theoretically in the same way as noise.

4. EXPERIMENTAL RESULTS

A 7L laboratory scale bioreactor acclimated with sludge taken from a municipal WWTP was used to degrade 4-chloro-phenol (4CP). The usual influent toxicant concentration for traditional sequencing batch processing is S_i=350mg4CP/L. Applying more than twice such quantity would greatly inhibit and stress biomass, increasing the needed treating time nonlinearly. Applying higher toxicant concentrations might even inhibit and/or disable the bioreactor permanently. By using the EDOC strategy, instead, the biomass was never stressed or inhibited. A linear increase relation of treating time with respect to S_i was observed in a series of experiments for increasing S_i, even when making it as high as 7000 mg4CP/L.

Theoretically, treating time was near 95% of the optimal-time, in all series, for a programmed $P = 0.9$

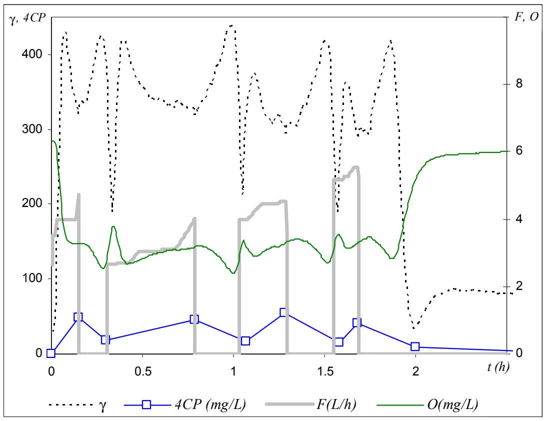

Figure 5. Experimental kinetics using EDOC in WWTP case 14/07/2003; $P = 0.9$; influent toxicant concentration $S_i = 634$mg4CP/L

Figure 5 shows one experimental kinetic for the 4CP degradation case, using y_w in Equation (8) for EDOC implementation. Toxicant substrate concentration S inside the bioreactor (see *4CP* in Fig. 5, square marks) was measured off-line from manually taken samples and was not used for control purposes. Up to S=200mg/L it is considered normal and safe for the biomass. A model identification exercise later revealed a 95% confidence interval of ±7.4% for $S^* = 13.99$ mg4CP/L. Figure 5 shows that S was kept oscillating around S^*, in an acceptably low concentration range, by properly turning *on* and *off* the influent pump (Fig. 5, continuous thick line). Such behaviour shows the effectiveness of EDOC strategy.

Biomass was B=1.4g exhibiting an increase of less than 2% during the reaction. Its value was not used by the controller. Values of S, S_i and S^* were not used either. Another perturbation comes from the online sensor used to measure Dissolved Oxygen (Fig.5, continuous thin line). It introduced appreciable second order delay effects, and some noise, to state variable O. It follows that some delays and signal distortion are to be expected when calculating $\gamma = y_w$ in Equation 8 (Fig. 5, dotted line) for using it in EDOC. But thanks to EDOC robustness the system did cope smoothly with all this perturbations and uncertainties.

5. CONCLUSIONS

A methodology for the robust and practical implementation of optimal control strategies for a class of nonlinear processes has been introduced. When the control law is composed of bang-bang and singular arcs the basic idea is to replace the singular arc with a bang-bang control. This makes the control robust and requires a reduced quantity of information. This general idea is developed here for a class of fed-batch bioreactors.

The use of measurable variables giving minimal indirect information is shown to be effective for software-sensing events related to the crossing of the singular surface of the process. This allows the controller to generate bang-bang cycles to approximate the singular arcs of the optimal solution.

Studies of two different practical cases were carried out successfully: one in the biotechnology area and other, including experimental results, in the wastewater treatment area.

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The scientific responsibility rests with the authors.

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Annex 03.WP5

EOLI
Efficient Operation of Urban Wastewater Treatment Plants

Work Package 5
Control Design and Application
Partner 6, UNAM
Mid-Term Report

Task leader
Jaime Moreno

Participants in this report

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May 2004

Contract Number ICA4-CT-2002-10012

TABLE OF CONTENTS

1. INTRODUCTION

This report presents the activities of the partner 6 (UNAM) concerning the WP5 of the EOLI project realized during the period November 2003-May 2004. In our case we investigate the control and optimization of the biodegradation of a toxic compound by naturally occurring microorganisms, i.e. WW1 and model EM1

2. PROBLEM FORMULATION AND JUSTIFICATION

Process Description

As a whole the process considered treats wastewater, which may include inhibiting toxicants, using an SBR (sequencing batch bioreactor). A series of stages must be executed in each batch of the bioreactor operation in order to have a complete treatment, i.e. Preaeration, Filling and Reaction, Sedimentation, Decantation, Purge (optional) and Standby (dead time, waiting for the next batch to start). From the control optimization and robustification point of view only the Filling and Reaction phase are considered of relevance.

The main treating process is related to the equation “reaction (1)”. This first reaction describes the degradation of the treated substrate via aerobic digestion.

$$Cl \cdot Phenol + O_2 \rightarrow X_1 + CO_2 + (metabolite) \qquad \text{reaction (1)}$$

$$(O_2 + metabolite \rightarrow X_2 + CO_2) \qquad \text{reaction (2)}$$

with X_1 and X_2 the corresponding biomasses for both reactions, respectively, and *Cl.Phenol* corresponding to the toxic inhibitory substrate.

Experiments have shown that metabolite is only produced if there is inhibition; otherwise there is only some weak quantity of metabolite. Moreover, it is not directly measurable. That is why the second reaction is not to be considered in the first approximation to design a controller for solving the problem.

Mathematical Model and Assumptions

The EM1 model (Carbon removal) is appropriate to the UNAM process. It is based on equation "reaction (1)" and it has the following dynamics while in the filling and reaction phase:

$$\dot{X} = \mu X - X\frac{Q_{in}}{V}$$
$$\dot{S} = -K_1\mu X + (S_{in} - S)\frac{Q_{in}}{V}$$
$$\dot{O} = -K_2\mu X - bX + K_l a * (O_s - O) + (O_{in} - O)\frac{Q_{in}}{V}$$
$$\dot{V} = Q_{in}$$

where X, S, O, V, K_1, K_la, S_{in}, Q_{in}, K_2, b, μ, O_{in} and O_s are biomass concentration inside the bioreactor, substrate concentration inside the reactor, Dissolved Oxygen (DO) concentration, water volume level of the reactor, biomass/substrate yield coefficient, oxygen mass transportation coefficient, influent substrate concentration, influent flow to the reactor, biomass/oxygen yield coefficient, specific endogenous respiration rate, specific biomass growth rate, influent DO and DO saturation value, respectively.

Some assumptions are in order for working in a laboratory setup, and them should be tested and revalidated once the field scale reactor is online. If some of the assumptions fail to comply, proper corrections should then be made to the control algorithms and software sensors.

Assumptions

1. Saturation DO remains constant throughout the reaction, i.e. the temperature inside the reactor is constant, and so is pressure and other factors that might alter its value.
2. DO level in the influent is neglectable
3. Aeration and biomass distribution are isotropic inside the reactor
4. Transport time is neglectable, i.e. the system can be modeled using ordinary differential equations instead of partial ones.
5. Biomass growth in one standard reaction is small, below 2%, i.e that the biomass concentration changes mainly only because of volume changes.

6. No biomass is added to the SBR, except when acclimating. EM1 does not model that.
7. No biomass is lost during decantation, except when purging. EM1 does not model that.
8. Biomass will not die appreciably during reaction time. EM1 does not model that.
9. *Kla* will vary with volume but not with substrate concentration.
10. For control purposes only the filling and reaction phase is of direct importance, hence no modelization nor special control is necessary for other phases as sedimentation, decantation, etc… This means that standard timed open loop control is used for the other phases.
11. μ is of the Haldane type or close to it. This means it grows monotonically from substrate concentration zero to some optimal substrate concentration S^*, where it takes the maximum value μ^*, and beyond that it decreases monotonically.
12. μ does not change, as a function of S, appreciably in one standard reaction.
13. DO concentration will remain above some given minimum concentration during a standard reaction. Failing to do so is interpreted as a sign of malfunction. This means no modeling for oxygen depletion is necessary for control purposes.
14. Before starting to fill, some preaeration will be allowed in order to fullfill the assumption above.

Definition of the Control Task and the Optimization Objectives

The control task is to obtain a nice cost/benefit relation for operating SBR to treat WW1. This implies a wise selection of instrumentation (sensors, actuators and controllers) combined with a clever utilization of control theory. In regard to this general objective the control theory may be used to obtain two desirable characteristics in the bioreactor's controller: Time Optimality and Robustness.

Optimality in time means more treated WW1 per time unit using the same resources, or equivalently using fewer resources to treat a given amount of WW1.

Robustification means that the controller should be able to work in near-optimal conditions even if mistakes are made when tuning it up, or if sensors are de-calibrated, or even if unexpected peak toxicant concentrations appear in the influent.

Expected Benefits from the Introduction of the Control Loop

Benefits arise, mainly, from two different reasons: Automation, Optimization and robustification.

Automation means that the decisions for operating the SBR are made autonomously by a computer using a control algorithm, disconnecting the human operator form the control loop. This makes it easier for the operator but the most important thing is that it allows the plant to be controlled in a repetitive and satisfactory way when normal conditions are presented, and to react quickly and appropriately to save the SBR when abnormal conditions arise.

Optimization of the process gives economic benefits in two ways. For WWTP yet to be designed, it allows to use less space, less materials and less investment for a given daily volume of treated WW1. For a plant already built and in operation, the addition of an optimal controller allows increasing the plant capacity without investing in another aspects other than the controller implementation.

Robustification offers various different benefits:

Robustness against unknown toxicant concentrations renders the benefit of allowing the bioreactor to survive, and even keep working optimally, when, for some unexpected reason, toxicant concentration peaks appear in the inflow. In practice this problem is the most frequent reason for SBR disabling. If this disabling happens, the reacclimation of an SBR may be a costly and time consuming task and, besides, all the WW will not be processed during this period and will probably pass untreated trough the system.

Robustness against uncertainties in model parameters allows the controller to work properly even if the operator or the technicians are not able to take correct measurements/calculations of the reactor parameters needed to tune up the controller.

Robustness against model uncertainty allows the system to work properly even if the real WW does not conform to WW1 or if the real SBR does not conform to EM1.

Robustness against calibration errors in sensors allows the system to work properly even if the data collected from sensors is biased and/or lacks linearity.

Control Validation Strategy (Theory, Simulations and Experiments)

The strategy for validating the proposed controller has 5 different and complementary stages. Initially a theoretical model of the control is built and formally tested using mathematical tools. Simultaneously a simulated controller based on EM1 is also build and tested using a wide range of parameter models to asses its robustness. Then a real-time controller is build and lab-tested using real WW1. Then the experimental results are taken to the simulator of the EM1 (without the controller) to see if the model reflects the real reactor when subjected to operation near the optimal point as the EDTOC theoretically does. Finally, a field test will be made with real WW1 and a field scale SBR.

To date only the last stage of the validation rests still unexplored. There are positive results in all other four stages.

3. DESCRIPTION OF THE PROPOSED CONTROL STRATEGY

The description of the EDTOC (Event Driven Time Optimal Control) strategy can be found in section 3 of Annex 01.WP5.

4. VALIDATION

Theoretical validation

This is done by assuring that if EDTOC (Event Driven Time Optimal Control) is used to control EM1, then the optimization objectives are, theoretically, reached. Mathematical work was done in various directions and the findings can be consulted in detail in section 3 of Annex 02.WP5

Description of Reactors and Equipment

The practical validation of the control strategy will be performed in two different experimental setups, for the reasons given in the Chapter on Problem Formulation and Justification. These two reactors are a Lab-Scale Bioreactor and a Field-Scale Bioreactor. The Field Scale reactor is in design process. The Lab-scale reactor is described next.

Lab-Scale Bioreactor:
A laboratory pilot reactor of 10L (7L of working volume) was used for the initial experiments. The reactor has a conical form to favor the settling of the sludge (Figure 1). The system of control was implemented using a personal computer and a data acquisition card (National instruments 6025E data acquisition card and the Labview package). An automatic temperature controller based on a recycle water pump was used to maintain a constant temperature close to 20^oC inside the reactor. The input and output water flows were controlled by the computed system using two peristaltic pumps (Cole-Parmer model 7523, Masterflex series), respectively. The computer controls a mixer and a gas mass flow controller (Cole-Parmer E-33116-20) that turned on the aerator from the bottom of the reactor. The aeration flow was 1.5 L/min for the standard condition. The synthetic wastewater contained 4-chlorophenol (4-CP) as carbon source and was complemented with nutrients the next composition per liter of water: KH_2PO_4 102 mg, K_2HPO_4 130 mg, $Na_2HPO4.H_2O$ 300 mg, NH_4Cl 30 mg, $MgSO_4.7H_2O$ 39 mg, $CaCl.2H_2O$ 63 mg, $Fe_2Cl_3.6H_2O$ 0.4 mg, $MnSO_4$-$2H_2O$ 0.003 mg, H_3BO_3 0.0057 mg, $ZnSO_4$-$7H_2O$ 0.0042 mg, $(NH_4)_6Mo_7O_{24}$ 0.0035, EDTA 0.0055 and $Fe_2(SO_4).6H_2O$ 0.0044 mg.

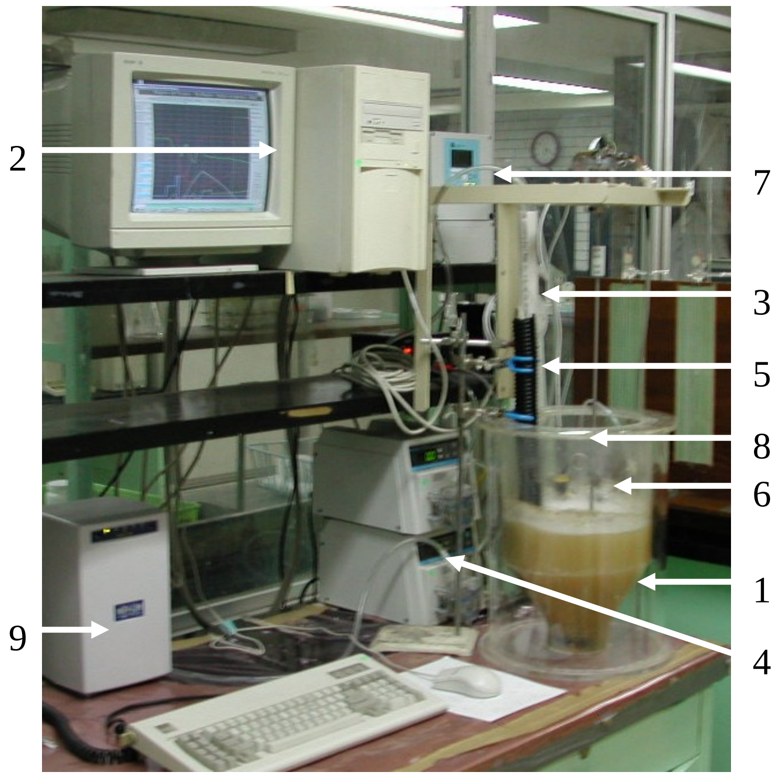

Figure 1. Pilot reactor utilized for the toxic compounds degradation. 1) Acrylic reactor with double wall and water recycling to maintain constant temperature at 20°C, 2) PC. 3) Acquisition card, 4) Peristaltic pumps (Master flex), 5) Temperature and Dissolved Oxygen Sensor (Endress + Hauser, COS4), 6) pH Sensor (Orion, model 720A), 7) Temperature and Dissolved Oxygen Transducers (Endress + Hauser, COM 223), 8) Level Sensor (Flow line LV10 series), 9) No break

The implementation of the control strategy

For implementing the control strategy, in simulation, SIMULINK and MATLAB were used. SIMULINK is a graphic oriented language. The program main window looks like Figure 2. Additionally MATLAB allows the building of friendly Graphic User Interfaces to communicate with the simulator. An example is shown in Figure 3.

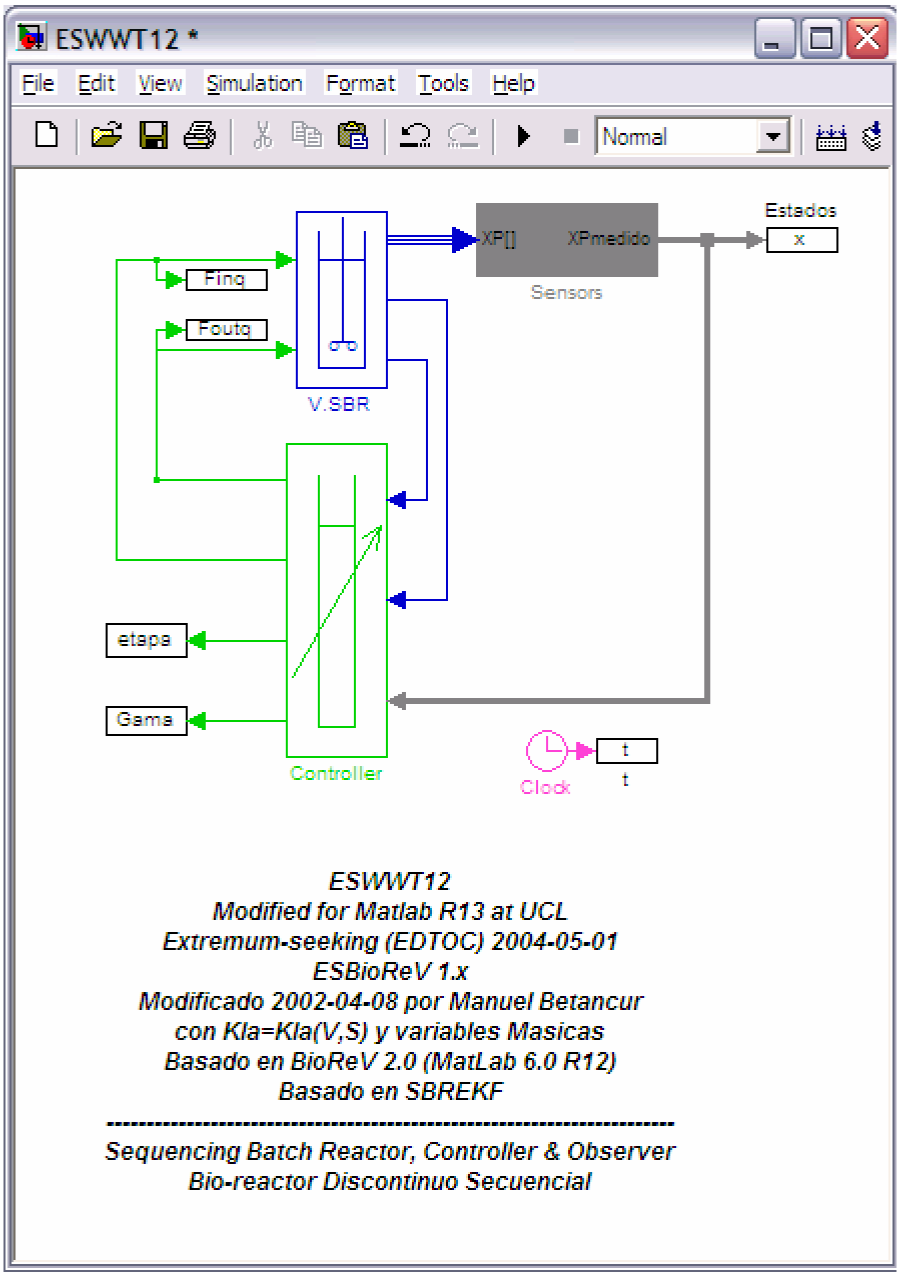

Figure 2. EM1 model and its controller programmed in SIMULINK

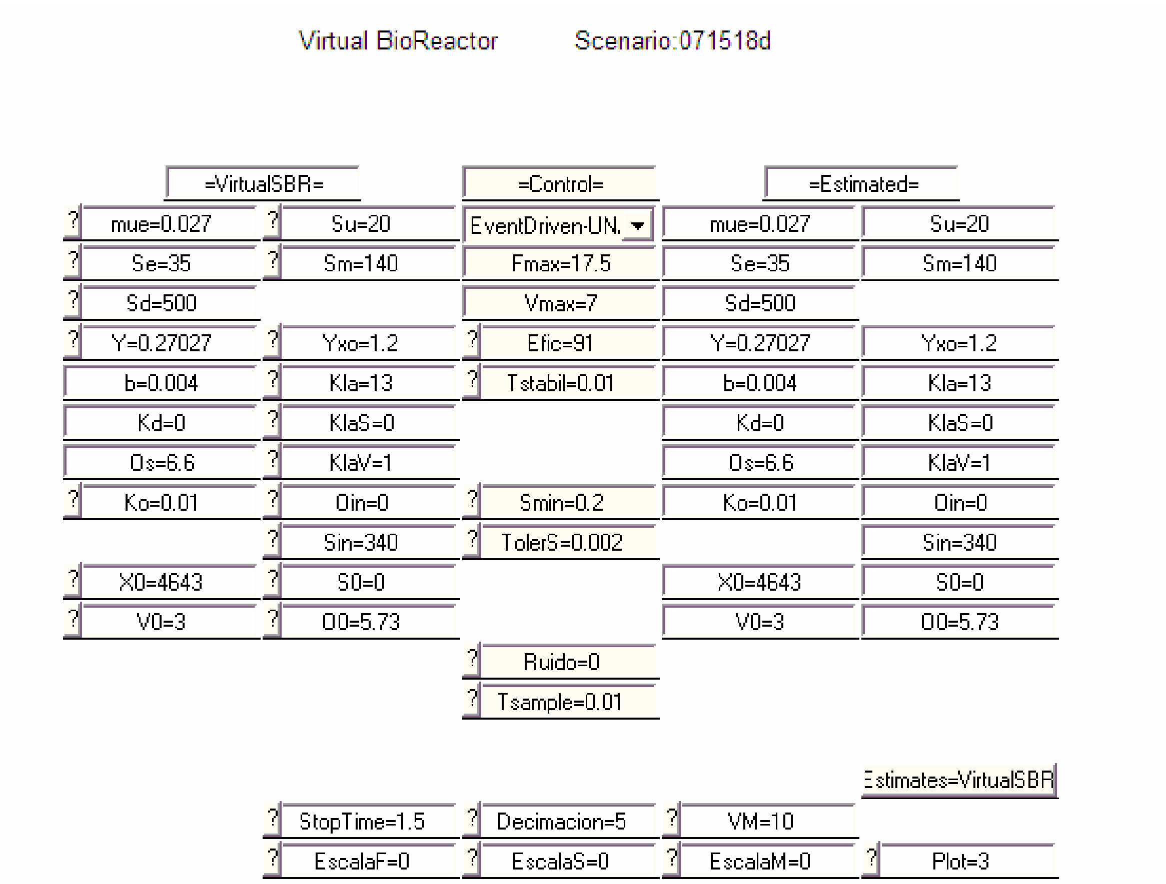

Figure 3. Graphic User Interface for using the SIMULINK simulator un MATLAB

To implement the controller in a real-time environment for use in laboratory LABVIEW language was used. LABVIEW is also a graphic oriented language. The front panel of the user interface with the program in the laboratory looks like Figure 4. The difference in both implementations reside in the fact that the real-time software has to cope with noise, uncertainties, bad sensor calibration and sensing delays, and is to be operated by technicians, while the simulator allows to control all the aspects of operation. This means the real-time program is more complex and more practically oriented. It includes all the phases for implementing a real reaction sequence, whereas the simulator only reflects the more important aspects of the process. Note that the language used in the front panel of the real-time application is Spanish and not English. The reason is that the operators are Spanish speaking persons and, using Spanish, the probability of misuse is reduced. Future versions may include English as the standard language.

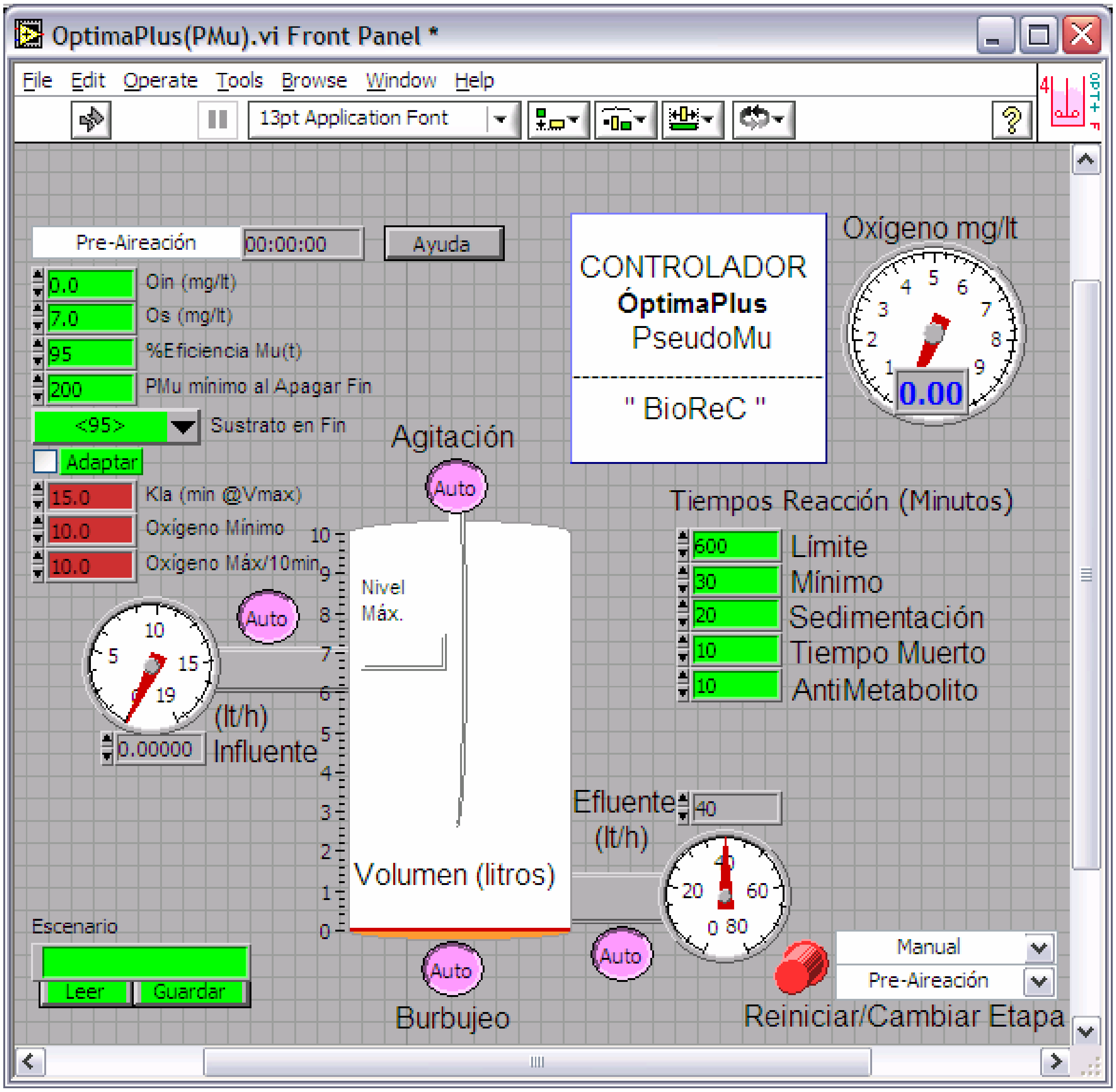

Figure 4. LABVIEW's Front Panel (Graphic User Interface) of the control strategy for operating the Lab-Scale real reactor

Experiments Conducted

A series of standard experiments using the EDTOC were conducted. The results are shown in figures 5 to 7. Different initial inflow values were tested. The EDTOC behaved acceptably in all of the experiments, but when the initial inflow was set to maximum the initial substrate overshoot was higher. After the initial overshoot all experiments behaved practically the same. In general, the properties of the reactions made using the EDTOC are as expected for standard toxicant concentration. However, there are not yet conclusive results for big substrate concentrations.

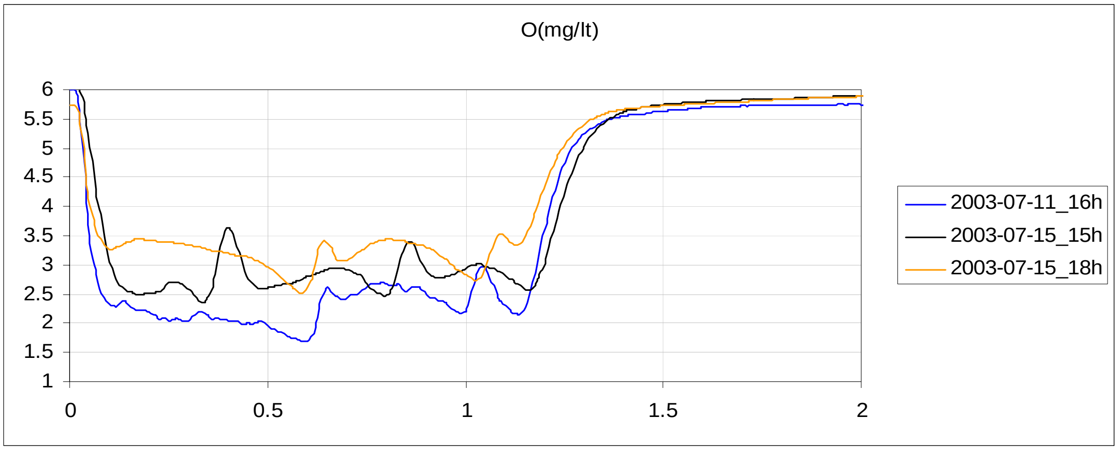

Figure 5. Different (3) DO kinetics for reactions using similar conditions and similar biomass. The most relevant difference is the (lower) initial inflow assigned to the controller in reaction 2003-07-15_15 (black)

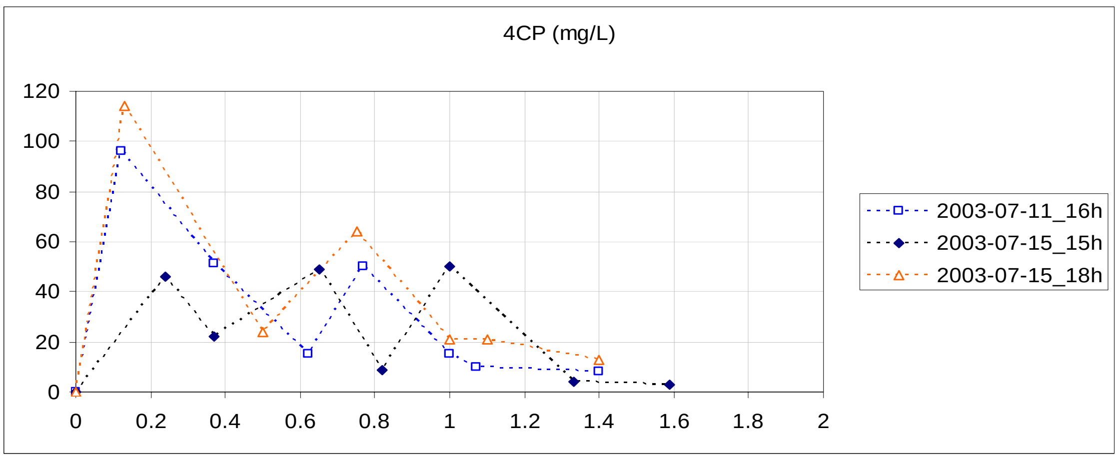

Figure 6. Substrate kinetics for same experiments as in Figure 5.

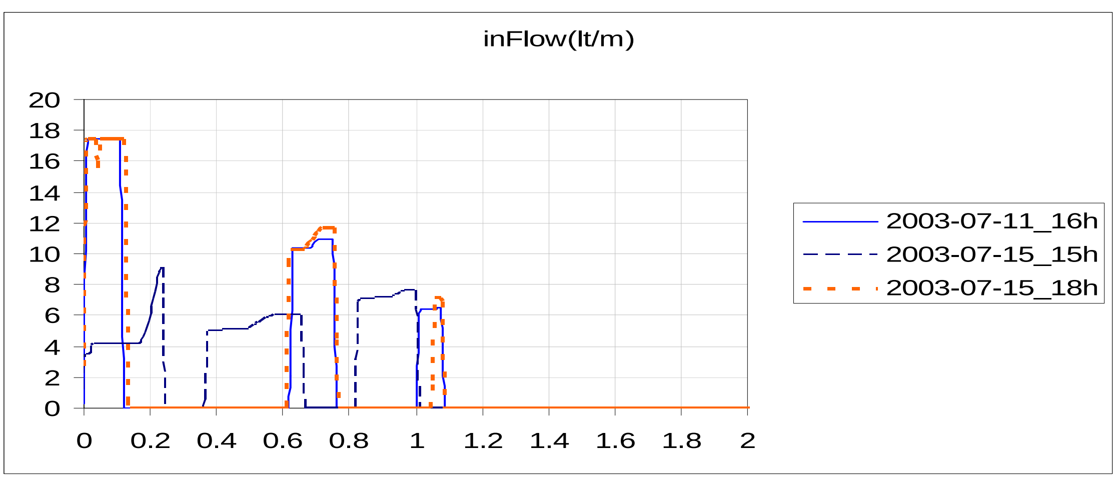

Figure 7. Inflow for same experiments as in Figure 5.

Simulations

Two kinds of simulations were conducted using WW1 and or EM1. The first series uses actual real data captured during the lab-scale experiments to feed the simulator. In this way the EM1 model is tuned to reflect in the best possible way the workings of the SBR. Once this tuning is made, the simulator is switched to total simulation mode and the second type of simulations are made. Those show how the control would behave in a perfect environment where the bioreactor follows the EM1 perfectly when treating WW1. Then, known variations in the parameters of the simulated plant could be made to test for robustness of the controller. Some of these simulations are presented in figures 8 to 12.

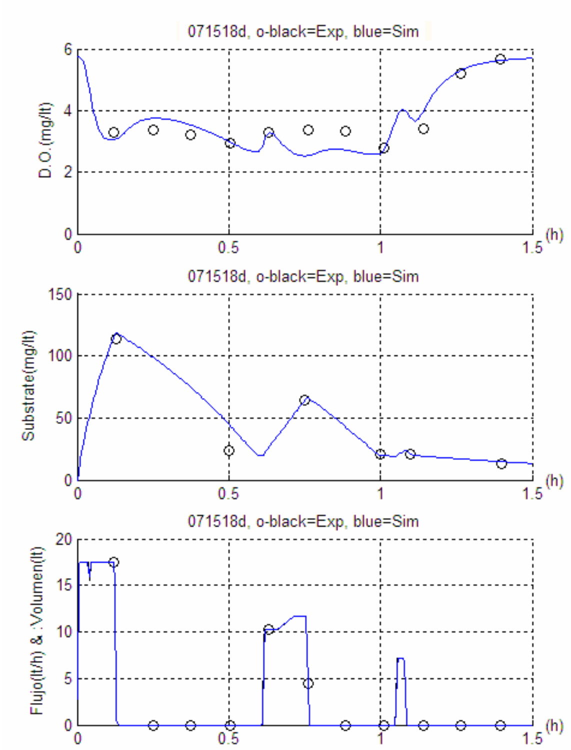

Figure 8. Simulated EM1, without control, fed with real input flow data (blue line) compared to real lab experiment (circles)

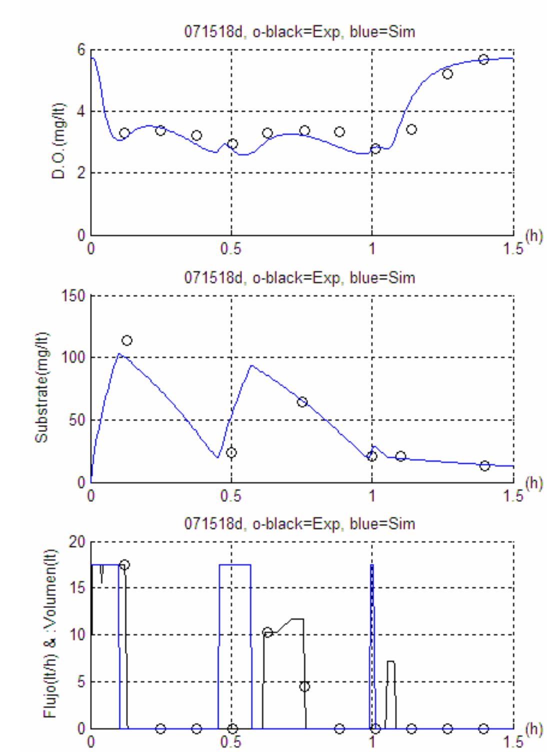

Figure 9. Simulated control (blue line) compared to real lab experiment (black circles)

Figure 8 was used to tune up EM1 as to reflect the behavior of the SBR when some given inflow is put into it (the same toxicant inflow the control did choose to apply in real experiment 2003-07-15_18h). The simulation results are compared against the results of the real experiment, obtaining a good match. After this is done, the same simulator is switched to ignore the given input and to decide, instead, its own input to the same experimental conditions.

Results of this second type of simulation are presented in figure 9. It can be seen that both, total simulation and real experiment, behave similarly. There are normal differences in

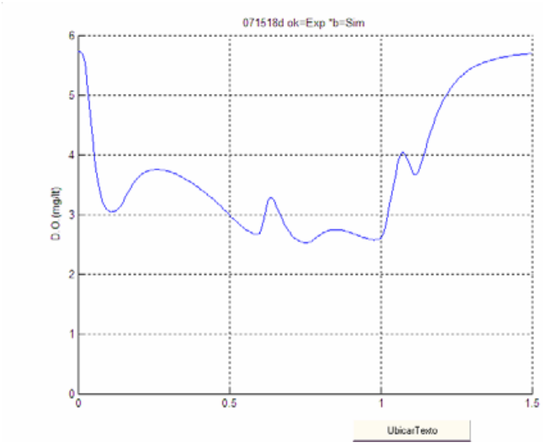

Figure 10. Simulated DO for real inflow 2003-07-15_18h applied to EM1

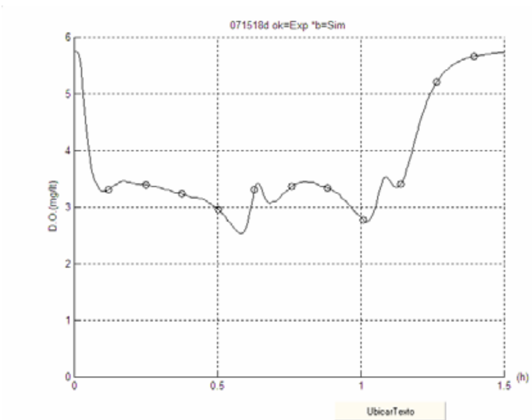

Figure 11. DO in real EDTOC lab experiment 2003-07-15_18h

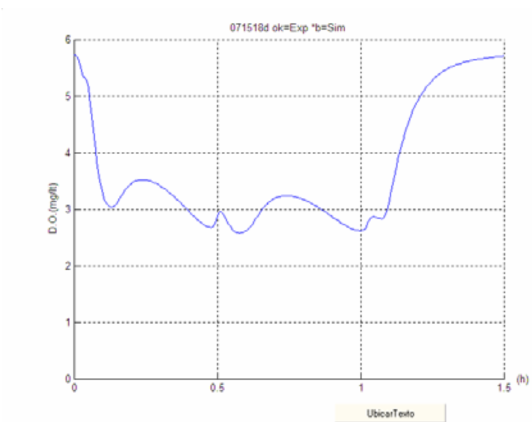

Figure 12. Simulated DO using ED-TOC with conditions similar to experiment 2003-07-15_18h

timing and absolute values, but shapes and all relative behaviors are virtually the same. This suggests that, although not exact, the simulator is an approximation good enough to use it in testing and validating the ED-TOC and, indirectly, to validate also the EM1.

DO kinetics are important for two reasons. First, it is the variable used by the software sensor to estimate the events in substrate and biomass growth. The controller uses such events to decide the influent rate. The second reason is that DO kinetics are harder to correlate to actual experimental data than substrate ones. This means that a good model will be such that correlates both of them and not only substrate. In fact, experience modeling EM1 shows that, a good DO behavior model invariable leads to a good Substrate behavior model.

Detailed DO kinetics are shown in figures 10 to 12 for comparison. It is easy to see that the shapes of all of them are similar. All of them show that the reaction required three (3) fill-wait sub cycles to complete, and they also show that oxygen demand remained at the same average level with sharp variations during filling and at the end of the waiting period, as predicted by EM1.

In all simulations a module for representing the sensor's time-delay was included. Originally such module was not present, an in fact is not modeled in EM1 equations but, after measuring experimentally such delay, it was found to be not neglectable. So it was added to the latest version of the simulator.

5. CONCLUSIONS

1. In simulation mode the EDTOC behaves exactly as predicted by the theory as long as no sensor noise or sensor delays are included in the EM1, i.e. it controls the reactor to operate it oscillating around but near the optimal zone (figures not shown).
2. In real experiments the substrate concentration goes higher than predicted in theory, but still the reactor oscillates around the optimal zone.
3. Once sensor delays are introduced in simulation mode, a better explanation of real data is obtained, and at the same time the simulated control exhibits a behavior in which it gets farther from the optimal zone, as real experiments do.
4. Sensor delays and sensor noise impose a practical limit on optimality, but this limit is not really restrictive and the process can be made more robust and optimal than the standard FTC mode, even for standard toxic concentration operation conditions
5. Once the sensor delay is incorporated to EM1, all DO kinetics do share the same shape in time, i.e. for pure simulation, for real-inflow in simulated EM1 and also for real experiments. The same observation holds for substrate.

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Aerobic treatment of toxic wastewater: problems, solutions, and open questions

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Abstract
The paper presents several attempts to solve the problems of concentration peaks and substrate starvation as well as the maintenance of a reliable performance of an aerobic sequencing batch bioreactor degrading toxic wastewaters. Two main solution lines have been followed: on one side, several control strategies, based on the measurement of the dissolved oxygen concentration, have been proposed. On the other side, the use of fixed biomass, or a mixture of suspended and fixed biomass, instead of suspended biomass has been pursued in order to overcome the problems mentioned above. It was observed that if no especial control strategy is designed the SBR systems with attached biomass have a better resistance against concentration peaks and toxic starvation than the suspended biomass systems. However, these solutions are not enough to increase sufficiently the performance of the SBR under extreme operating conditions. I was observed that sophisticated control strategies as the time optimal control greatly increased the robustness and performance of the SBR to levels never obtained before without them.

Keywords: optimal control, dissolved oxygen, 4-clorophenol, starvation, toxic peaks, moving bed, suspended biomass.

INTRODUCTION

The biological treatment of toxic wastewater with high concentrations of toxic compounds, such as that produced by the chemical and petrochemical industries is a difficult and challenging task. Aerobic sequencing batch reactors (SBR) have demonstrated their superiority with respect to the continuous reactors due to their better efficiency and flexibility. The term SBR is used as a synonym of the wastewater treatment technology, where the volume of the reactor tank is variable in time (Wilderer et al. 2001). It can work with suspended or attached biomass. In general, the SBR process presents three major characteristics: periodic repetition of a sequence of well defined phases; planned duration of each process phase in accordance with the treatment result to be met, and progress of the various biological and physical reactions as a function of time. Another characteristic of SBR systems, because of their flexibility in control strategy, is that they are effective for fully automated computer controls.

However, standard operation modes of SBRs face several key problems in the treatment of toxic wastewaters:

1. The behavior under sudden increase of the toxic substrate concentration (concentration peaks) in the wastewater that severely affects the operation of the wastewater treatment plant (WWTP). They are frequent because of intermittent industrial operation, that generates concentration peaks when, for example, the containers and reactors are cleaned.
2. The toxic nature of the substrate makes it necessary to previously acclimate the biomass for degrading the toxics. Moreover, the exposition of the acclimated population to prolonged periods of starvation, usual under common SBR operation policies, produces a decrease of the bacterial activity and, even the death (Coello *et al.*, 2003; Buitrón and Moreno 2002). This problem is usually not taken into account in the operation of biological WWTPs.
3. The adequate control of the SBR requires the on-line monitoring of the toxic concentration in the reactor. However, this is not practically and economically implementable at a WWTP level. To overcome this problem several operation modes have been proposed using either the carbon

dioxide evolution rate (Buitrón et al. 1993) or the dissolved oxygen (DO) concentration (Sheppard and Cooper, 1990). They proposed a control strategy, called Self-Cycling Fermentation (SCF), in which the length of the growth period is controlled by the biological activity in an aerobic reactor, and based on the close correlation between DO concentration in the reactor and cellular respiration.

4. The treatment of toxics decreases the time efficiency of the plant, since an increase in the toxic concentration increments the reaction time in a not proportional manner.

The objective of this paper is to present several attempts of our research group to solve these problems. Two main solution lines have been followed: on one side several control strategies, based on the measurement of the DO concentration, have been proposed. On the other side the use of fixed biomass, or a mixture of suspended and fixed biomass, instead of suspended biomass have been pursued in order to overcome the problems of starvation and concentration peaks, and in view to maintain a high efficiency of removal of toxic contaminants as well as a reliable performance of the system. The results of these proposals will be discussed, and some open problems will be presented.

METHODOLOGY

Pilot reactor

A pilot system with an aerobic reactor of 7 liters of useful volume (Figure 1) was employed to treat synthetic wastewater containing 4-chlorophenol (4CP) or a mixture of phenolic compounds in an equal proportion (phenol, 4CP, 2,4-dichlorophenol, and 2,4,6-trichlorophenol). Nutrients such as nitrogen, phosphorus, and oligoelements were added following the techniques recommended by ANFOR (1985). The pH was maintained around 7.0. The substrate concentration was measured taking samples and processing them offline using colorimetric techniques with 4-aminoantipyrine method (Standard Methods, 1992). To determine the biomass concentration at a given instant, total and volatile suspended solids (VSS) analysis was made (Standard Methods, 1992). Dissolved organic carbon (DOC) analysis was also performed to test whether 4CP was being mineralized (Shimadzu TOC-5050). The exchange ratio in the reactor was 4/7 and the airflow is 1.5 liters per minute. An automatic temperature controller based on a recycling water pump was used to maintain a constant temperature of 20 oC inside the reactor (PolyScience model 210). Dissolved oxygen was measured using an electronic meter (YSI model 52) coupled to a computer. The input and output water flows were controlled using peristaltic pumps, which could be read and controlled by the computer (Cole-Palmer model 7523, Masterflex series). Additionally, the computer could also control a mixer and a valve that turned on the aerator. The treatment process used is SBR type with 5 steps: filling, reaction, sedimentation, decanting and an idle period.

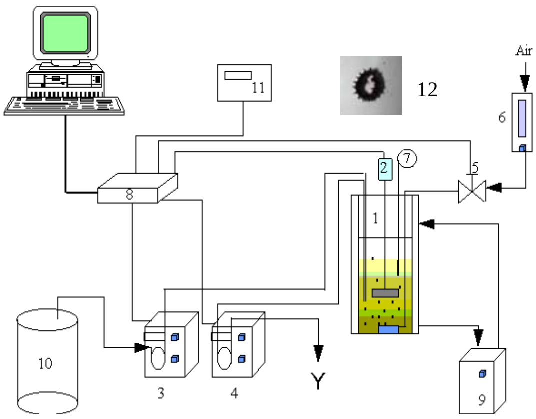

Figure 1. Experimental assembly. Reactor (1), mixer (2), feeding pump (3), drawing pump (4), flow controller (5), flowmeter (6), thermometer (7), interface (8), flow-through heater (9), storage tank (10), oxymeter (11), packing material used in the moving bed (12).

Biomass

The reactor was inoculated with microorganisms coming from a municipal activated sludge treatment plant (2000 mgVSS/L). A cell retention time of 20 days was maintained. The biomass was used considering 3 alternatives: Suspended Biomass (SB), a Moving Bed system (MB), which is composed by a mixture of suspended biomass and fixed biomass previously colonized in a polyethylene packing of high density (BCN009 plus from the 2H company, with a superficial area of 963 m2/m3), and Fixed Biomass (FB) being the packing material a porous volcanic rock (puzolane) with a mean diameter from 1.0 to 1.5 cm and 63% of porosity. The biomass was acclimated using the fixed timing control strategy before appliying any of the strategies discused later. Acclimation was done to an initial concentration of 50 mg/L in the reactor. When degradation times were constant, the initial concentration was stepwised incremented up to 200 mg/L in the reactor (350 mg/L in the feed tank). In the case of the mixture of phenos an initial substrate concentartion of 175 mg/L (100 mg/L in the reactor) was used.

Strategies used for controlling the operation of the SBR

Different control strategies can be used to control the fill and reaction phases of the SBR: *Fixed Timing Control* (FTC) is the usual control strategy in the WWTP, *Variable Timing Control* (VTC) (Buitrón et al., 2003), *Time Optimal Control Observed Based* (OB-TOC) (Vargas et al., 2000) and *Event Driven Time Optimal Control* (ED-TOC). Next, we explain each one of them. The simplest one is the FTC, which has the same layout as the VTC in Figure 2a1, except that it lacks a *reaction's near-end detector* (RNED). However, their Volume-Substrate plane trajectories (VSpt) are identical (see arrows path in Figure 2a2). This VSpt means that, when a batch starts, the SBR is filled quickly and the substrate concentration ($\boldsymbol{S}$) raises from zero to $\boldsymbol{S}_b$ (or S_o) value inside the inhibition zone. The substrate biodegradation then starts slowly (see detail in Figure 2a2). Note that a horizontal trajectory means there is no filling going on. The FTC will end that reaction based on a fixed timing, regardless of the $\boldsymbol{S}$ left. The VTC, instead, will end it based on the dissolved oxygen ($\boldsymbol{O}$) behavior. Its RNED alerts the *sequencer timer* (ST) when the oxygen consumption quickly decays to a value associated to a metabolic state explained by $\boldsymbol{S}\leq\boldsymbol{S}_f$. Then some extra time is allowed for the reaction to finish. The ST decides the timing for all of the batch stages, and also decides when to fill, apply air, stir and decant the SBR. The flow values are preset in the ST, as are also the timer values for all stages. The only automated variable timing is the reaction time. For such action the VTC and the *time optimal controllers* (TOC) do have a RNED embedded, thus guaranteeing that the reaction will be ended in due time.

The TOC mode VSpt is shown in Figure 2b2 (Moreno, 1999). This operation mode aims at filling the reactor quickly to the optimal concentration $\boldsymbol{S}^*$, and then apply an inflow rate $\boldsymbol{Q}_{in}=\boldsymbol{Q}_{opt}$ just enough to keep $\boldsymbol{S}=\boldsymbol{S}^*$. Hence, the vertical trajectory, meaning there is no change in $\boldsymbol{S}$ while $\boldsymbol{V}$ increases. If $\boldsymbol{S}$ could be measured, doing this would be easy for a standard controller. However, as it is not, the *observer based* (OB)-TOC (Vargas *et al*., 2000) in Figure 2b1 solves this theoretically, by estimating $\hat{S}\approx\boldsymbol{S}$ using $\boldsymbol{O}$, $\boldsymbol{V}$ measures. An observer derived from the SBR mathematical model does this. The drawback is that it needs to know exactly the inflow substrate concentration ($\boldsymbol{S}_{in}$) and other critical SBR parameters as $\boldsymbol{S}^*$. A slight mistake in estimating such parameters renders the observer useless and then the real VSpt will not resemble Figure 2b2. This makes the OB-TOC very difficult and unreliable to apply.

The *Event Driven* (ED)-TOC (Betancur *et al.*, 2004) in Figure 2c1 solves the problems by not looking at $\boldsymbol{S}$, but instead finding a variable (named γ) related to the reaction's speed. Such γ can be estimated in real time by using $\boldsymbol{O},\boldsymbol{V}$ measures in formula (1). Compare γ and μ in Figure 2c2 and Figure 2b2. They do have the same shape. That is why it is feasible to control $\boldsymbol{Q}_{in}$ so that the reaction's speed stays inside the *fast zone* in Figure 2c2. Such zone is above a ***P%*** of the maximum speed. Associated with that there is a shaded rectangle to explain how controlling the speed indirectly keeps the unknown $\boldsymbol{S}$ oscillating in a gap between some $\boldsymbol{S}_{pl}$ (lower than $\boldsymbol{S}^*$) and $\boldsymbol{S}_{ph}$

(higher) all the way trough the SBR filling. Every time $\boldsymbol{S}$ tries to leave this gap, an event is issued and the ED-TOC then switches $\boldsymbol{Q}_{in}$ on/off, to prevent it. This is why the VSpt zigzags inside the shaded envelope. As $\boldsymbol{P}\rightarrow 100\%$ the zigzags will be finer and then the ED behavior will approach the theoretical TOC. This will work regardless of the $\boldsymbol{S}_{in}$ value and despite changes in most of the SBR parameters. Only $\boldsymbol{K}_l a$ and $\boldsymbol{O}_s$ are needed to estimate γ and they do not even need to be known precisely. This makes the ED-TOC robust. In control terms, this means that increasing the error in obtaining those parameters will only degrade the ED-TOC performance gradually. Even when those parameters are badly given, the ED-TOC will behave acceptably. This solution is therefore a good candidate for uses in real industrial environments.

$$\gamma \overset{\Delta}{=} \frac{B}{Y_{X/O}}\mu + bB = K_l a\left(O_s - O\right)V - OQ_{in} + \frac{dO}{dt}V \qquad (1)$$

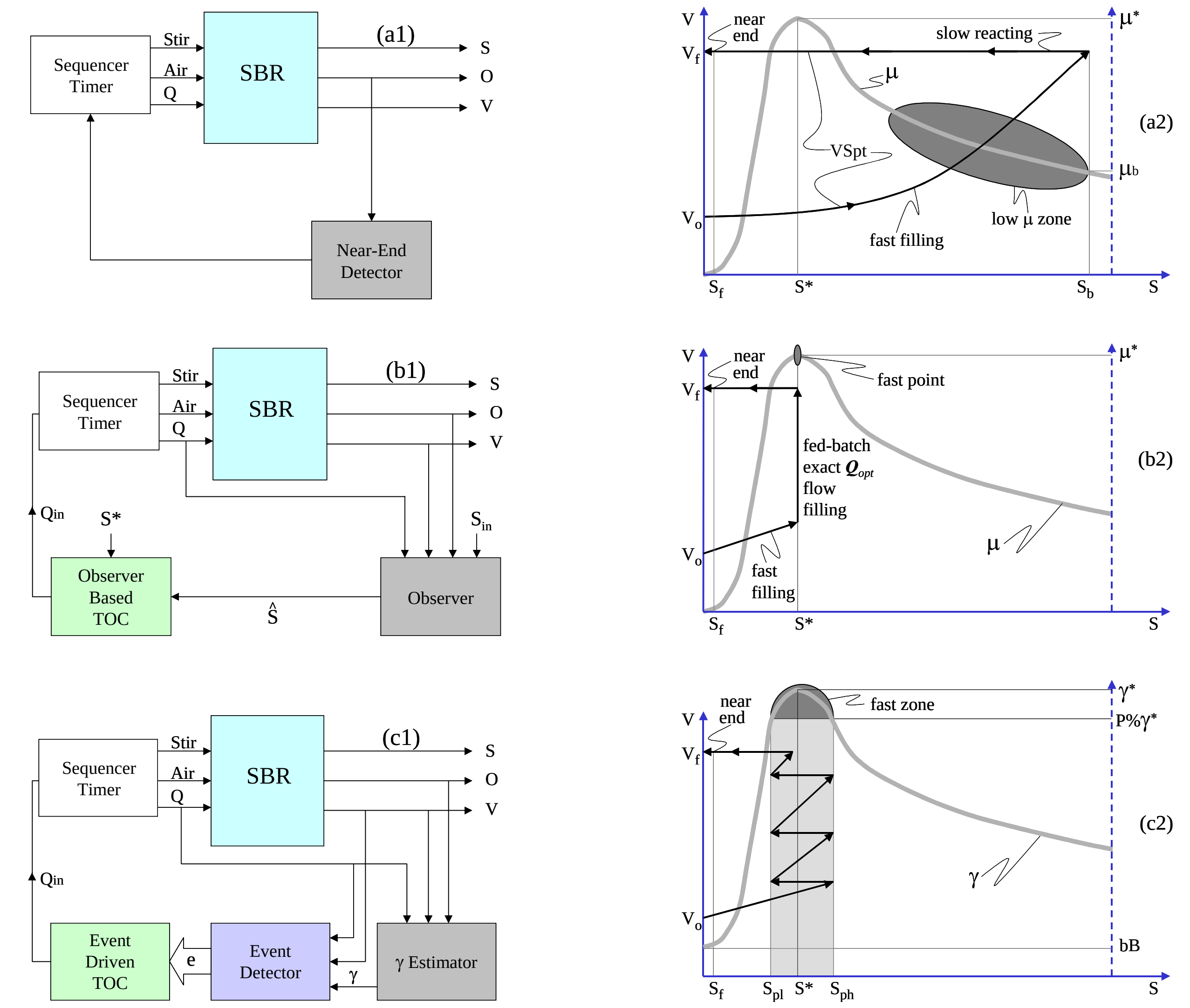

Figure 2. a) VTC, b) OB-TOC, c) ED-TOC; 1) Control Layout, 2) V-S plane trajectory (VSpt); Secondary dashed axis for □ or □ respectively. A dark area marks the speed related zone in which the process spends most of its time. Initial $\boldsymbol{S}$=0 and $\boldsymbol{V}=\boldsymbol{V}_o$ conditions are assumed.

Experimental strategy

The main problems identified, as susceptible to be solved, were: lack of robustness of the SBR when confronted to peak substrate concentrations (PSC), loss of activity due to starvation (LOS), and variations in degradation efficiency (DE) because of operating into the inhibition zone. It would be also desirable to test the long-term stability (LTS) of the new solutions.

For testing possible solutions to these problems, a series of experiments in two different directions were conducted. The main philosophy is to increase complexity step-by-step, beginning with the simpler modes. Future experiments (FE) will combine this two research axes. Table 1 shows the experimental strategy.

Table 1. Experimental strategy based on two different research directions. The problems to be solved in each case are referenced. Future experiments (FE) are also suggested.

Control modes / Biomass configurations	FTC: Fixed Timing Control	VTC: Variable Timing Control	OB-TOC: Observer based Time Optimal Control	ED-TOC: Event Driven Time Optimal Control
SB: Suspended Biomass	SOC PSC LOS DE	PSC DE	PSC DE FE=LTS	PSC DE FE=LTS
MB: Moving Biomass	PSC LOS DE	FE=All	FE=All	FE=All
FB: Fixed Biomass	PSC LOS DE	FE=All		

In order to obtain comparable data for testing the different control modes, a standard operation condition (SOC) was defined. For doing any control mode experiment, the reactor was previously running in SOC. Then the experimental kinetics is made and, after that, again a SOC is conducted. This allows comparing the "after" and "before" SOC kinetics to asses the short term impact of the new mode in the SBR parameters.

RESULTS AND DISCUSSION

Note that the initial concentration condition is reported in two forms. The influent substrate concentration present in the storage tank and fed to the reactor is called S_{in}. Once the reactor was fed, the influent substrate concentration becomes the initial substrate concentration (S_o) and depends on the internal dilution (or the volume exchange ratio). Removal efficiencies of 4CP and the mixture of phenols were always superior to 98%, except for the days when the perturbations were introduced (concentration peaks or starvation). Degradation rates were computed taking into account the quantity of substrate degraded, and dividing this by the quantity of VSS and the filling and reaction times. During acclimation degradation rate (q) varied from 20 to 60 mg 4CP/gVSS-h, for the suspended biomass. The sludge volumetric index (SVI) obtained was in average 40 mL/g, indicating the excellent characteristics of the sludge. MLVSS concentration varied between 1800 and 2500 mg/L, as a consequence of the daily purge of sludge to maintain a mean cell retention time of 20 d. Mean concentration was 2000 mgVSS/L.

Once the biomass was acclimated, the reactor was operated under a determined strategy. Decanting (30 min), idle period (15 min) and drawing (15 min) times were always the same no matter the type of biomass or control strategy used. In the case of the FTC, filling time was 15 min, and reaction time was fixed in 4 h. When a peak was introduced under this control strategy, reaction time was increased to allow as much as possible the phenol(s) degradation. Figure 3a presents the behavior of a cycle operated under the VTC strategy using 4CP as substrate. For this case filling time was 15 min. After an extra time of 20 min, the reaction was stopped. When a concentration peak was introduced, the system searched for the minimal DO concentration in order to determine the end of the reaction phase. When the TOC strategy (either for the OB and EV modes) was implemented, filling rate was the necessary to maintain the substrate concentration at S*; thus reaction and filling phases occurred simultaneously. At the moment when the maximal volume was reached, the filling phase stopped and only reaction phase occurred. When a concentration peak was introduced, the algorithm determines the optimal influent rate allowing the necessary time to biodegrade the volume of the toxic water. Figure 3b presents an example of the DO and toxic evolution in the reactor during a concentration peak of 5200 mg4CP/L, with the ED-TOC strategy.

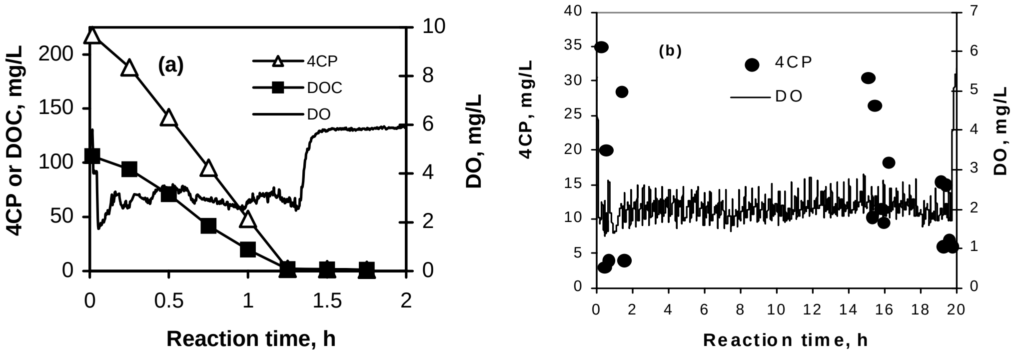

Figure 3. Evolution of substrate concentration and dissolved oxygen for the VTC (a) and the TOC-ED (b) strategies.

Effect of the concentration peaks

Table 2 summarizes the effect of the concentrations peaks on the performance of the reactor. For all the cases, the best performances were obtained with the ED-TOC strategy. Maximal initial peaks concentrations were degraded with this strategy. Thus, it was possible to degrade S_{in} concentrations up to 11200 mg 4CP/L. Theoretically there is not limit in the initial concentration since the algorithm always will keep the concentration al the optimal value. With the usual control system, based on fixed times, the worst performances were observed. Only 550 mg/L was possible to biodegrade with 100% of efficiency removal. However, it is interesting to point out the promissory results obtained with the moving bed. If the MB and SB are compared using the FTC algorithm, it is observed that the mixture of attached and suspended biomass generates better results than the suspended biomass alone. Up to 1850 mg4CP/L were possible to treat without problems in the degradation efficiency (almost 3 times more than the SB system).

Comparing the degradations rates obtained before the concentration peaks it is noted that using the time optimal control strategies (OB and ED) it was possible to obtain the highest rates of the system. Taking an equivalent fed concentration of 700 to 850 mg 4CP/L, 79, 60, 33 and 25 mg4CP/gVSS -h values for the degradation rate were obtained when the reactor was operated under the TOC, VTC, FTC-MB and FTC-SB strategies, respectively. For this range of fed concentrations, the MB presented better results than SB for similar concentrations.

The major impact of the toxic peaks was observed just after the peak for the FTC control strategy. When a new cycle was conducted (at 350 mg/L), the degradation rate obtained with the FTC-SB after the 900 mg/L peak decreases 80%. That means that a waste water treatment plant will need five times more time to degrade the usual influent concentration. On the other hand, the degradation rates were not affected after a sudden introduction of a toxic shock load when the reactor was operated under the time optimal control strategy. Even, in some cases when the *event driven* algorithm was used a higher degradation rate was obtained (114 mg 4CP/gVSS -h) during the peak.

Effect of starvation periods

When a given biomass was acclimated to a toxic compound, present in an industrial effluent, is subject to starvation periods against the toxic (no to the easily biodegradable substrate), there exist a lost of activity (Buitrón and Moreno, 2002). This implies that the efficiency of the treatment would be affected when the toxic enters again to the WWTP. Figure 4 presents the effect of starvation periods on the performance of the reactor when suspended, fixed and a mixture of suspended and fixed biomass is used. It is clear the beneficial impact generated by the fixed biomass. When a mixture of phenols was used, there is only 35 % of increment in the degradation time (against almost 100% for suspended biomass). In the case of 4CP, the impact of starvation is avoided clearly by the use of the carrier material, indicating again the robustness of the process by the attached biomass (Gheewala and Annachhatre, 2003).

Table 2. Effect of different operational strategies on the reactor performance under peaks of concentration.

Control strategy	Type of Biomass	Peak of 4CP, mg/L (S_{in})	Efficiencies during the peak (%)	Degradation rate before the peak (mg 4CP/gVSS-h) **qb**	Degradation rate during the peak (mg 4CP/gVSS -h) **qd**	Degradation rate after the peak (mg 4CP/gVSS -h) **qa**	Degradation rate ratio after the peak **(qa/qb)**
FTC	SB	550	100	25.0	21.0	22.2	0.9
		760	85	25.0	18.5	11.3	0.5
		900	63	25.0	21.4	7.4	0.2
FTC	MB	850	100	33.3	44.4	33.3	1.0
		1850	100	33.3	24.3	26.7	0.8
		3240	20	33.3	6.9	N.D.	N.D.
VTC	SB	700	100	59.8	44.9	59.8	1.0
		1050	100	59.8	9.0	18.0	0.3
		1400	18.3	59.8	0.9	N.D.	N.D.
OB-TOC	SB	700	100	79.3	57.1	79.3	1.0
		1050	100	79.3	45.1	79.3	1.0
		1400	100	79.3	73.3	79.3	1.0
ED-TOC	SB	700	100	71.4	63.5	71.4	1.0
		1400	100	65.0	91.2	71.4	1.1
		2800	100	95.3	114.3	101.5	1.1
		5600	100	81.6	114.3	71.4	0.9
		11200	100	71.4	114.3	64.5	1.0

N.D. Not enough degradation was archived to compute the degradation rate

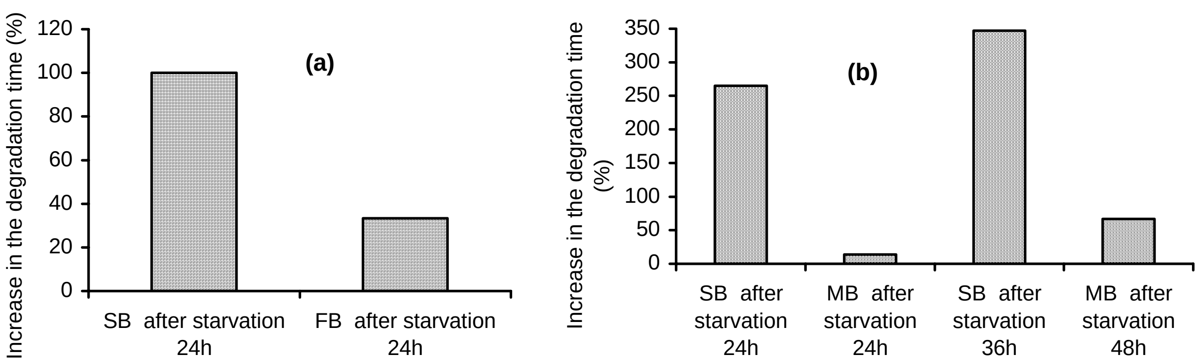

Figure 4. Increase in the degradation time due to different starvation times, in respect to the degradation time observed before starvation: (a) 100 mg/L of mixture of phenols (25 % each), (b) 100mg/L of 4-CP. Degradation times (in hours) were (before and after): (a) SB 24h (1.23, 4.5), FB 24h (3,4) and (b) SB 24h (2, 4), MB 24h (1.5, 1.71), SB 36h (1.23, 5), MB 48h (1.5, 2.5).

CONCLUSIONS

From the results obtained so far, two important results are easily seen:

1. If no especial control strategy is designed (let say FTC strategy) then SBR systems with fixed biomass (MB or FB) have a better resistance against concentration peaks and toxic starvation than SB systems. However, these solutions are not enough to increase sufficiently the performance of the SBR under extreme operating conditions.
2. Sophisticated control strategies as OB-TOC, and specially ED-TOC, greatly increase the robustness and performance of the SBR to levels never obtained before without them. The investigation in developing such control modes is, therefore, very promising.

Several experiments have to be done to finalize this study. Long-term Stability of the SBR under the TOC strategies has to be studied, before a strong affirmation about their properties can be done. This includes specially the study of the evolution of the properties of the biomass under such control strategies. Our hypothesis is that the combination of suspended and fixed biomass (Moving Bed) with the Time Optimal Control strategy will give the best results in terms of efficiency and robustness of the whole system. This is part of the future work.

AKNOWLEDGEMENTS

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EVENT SOFTWARE SENSOR AND ADAPTIVE EXTREMUM SEEKING ALTERNATIVES FOR OPTIMIZING A CLASS OF FED-BATCH BIOREACTORS

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Abstract: Optimization and control in spite of plant uncertainties is always a challenge, especially if additional constraints about measurements are present. Here, two different approaches to solve this problem are compared using simulation. They aim at reducing the operation time of bioreactors with inhibitory behavior where measuring the reaction rate is not feasible. The “Adaptive Extremum Seeking” proposed version relies on the structure information of the kinetic model and requires the measurements of the substrate and one other related variable. The “Event Driven Time Optimal Controller” strategy avoids the substrate measurement and, using an event software sensor, provides a nearly optimal solution without requiring a complete model. *Copyright © 2004 IFAC*

Keywords: Extremum seeking, software sensor, optimal control, fed-batch bioreactor, Haldane kinetics, control applications, biomass production

1. INTRODUCTION

The performance of fed-batch fermentation processes could typically be increased by the use of model-based optimization techniques. Using a fairly general model structure, many useful results have been derived in (Modak et al., 1986; Van Impe et al., 1994). One key result is that, in many cases, the final product yield (ratio of the amount of product formed and the amount of substrate consumed) can be maximized simply by maximizing the instantaneous yield. This can be achieved by maintaining the substrate concentration at an optimal level called S^*.

Over the past years, significant research effort has been done in the real time optimization for fed-batch bioreactors. The primary objective has been to overcome the performance limitations associated with the large uncertainty related to models of these processes (e.g. Bastin and Dochain, 1990).

In this paper, two approaches that are aimed at handling the uncertainties on the process kinetics are comparatively investigated. The version of the Adaptive Extremum Seeking (AES) proposed here utilizes explicit structure information of the objective function that depends on system states and unknown plant parameters. A Lyapunov-based adaptive control technique is used to estimate the unknown kinetic parameters and to drive the system to its unknown extremum. The second approach, the Event Driven Time Optimal Control (ED-TOC) uses bang-bang techniques based on the optimal solution approach, solving the problem without measuring the substrate nor needing the exact structure of the model.

The paper is organized as follows: in Section 2 the problem is stated. Sections 3 and 4, respectively, present the ED-TOC and the AES. A comparative simulation study is done in Section 5. Some conclusions and perspectives close the paper.

2. PROBLEM FORMULATION

In this work, we consider the optimization problem for a class of simple microbial growth processes with one gaseous product in a fed-batch bioreactor, described by the following dynamical model:

$$\frac{dX}{dt} = \mu X - DX \tag{1}$$

$$\frac{dS}{dt} = -k_1 \mu X + D(S_i - S) \tag{2}$$

$$y = k_2 \mu X \tag{3}$$

$$\frac{dV}{dt} = DV \tag{4}$$

where states *X (g/L)* and *S (g/L)* hold for biomass and substrate concentrations, respectively, μ *(h^{-1})* is the specific growth rate, $D = \frac{F}{V}$ *(h^{-1})* is the dilution rate, *y (g/L/h)* is the production rate of the reaction product, S_i *(g/L)* denotes the concentration of the substrate in the feed, k_1 and k_2 are yield coefficients, *F (L/h)* is the inflow and *V (L)* is the volume of the liquid medium in the tank.

A Haldane law approximates the specific growth rate:

$$\mu = \frac{\mu_0 S}{K_S + S + S^2 / K_I} \tag{5}$$

Where μ_0 is a parameter related to the maximum value of the specific growth rate μ^*, K_S denotes the saturation constant and K_I the inhibition constant. Such a model is typically used to describe the substrate inhibition effect in fed-batch bioreactors, as shown in Figure 1.

The control objective is to produce the maximum amount of biomass in the minimum possible time. It is well known (Moreno, 1999) that this will be achieved if μ is kept at its maximum value, μ^*, as shown in Figure 1.

3. EVENT DRIVEN TIME OPTIMAL CONTROL

The ED-TOC is based on the time optimal control solution to the problem (Moreno, J. 1999), which consists of bang-bang arcs and a singular arc. The

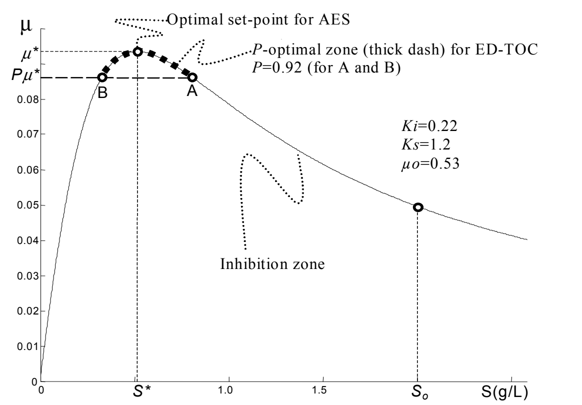

Figure 1. Haldane's type biomass specific growth rate

singular arc maintains $\mu=\mu^*$ using a continuous control function, for which a good knowledge of the model would be required. The ED-TOC does the bang-bang arcs exactly but it approximates the singular arc by a switching strategy. This allows operating as near to the optimum as desired without the necessity of measuring many state variables and with a high degree of robustness against model and parameter uncertainties and changes. It considers also the physical restrictions of the actuator.

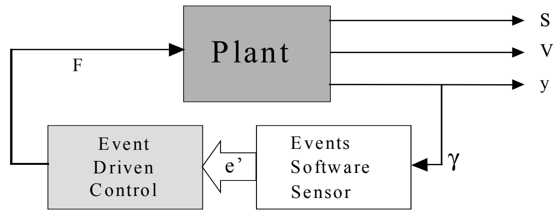

Figure 2. ED-TOC scheme

The ED-TOC estimates if μ lies inside a *P*-optimal zone, depicted in Figure 1, and acts accordingly to keep it inside. Figure 2 shows the ED-TOC scheme (a formal description is available in Betancur et al. 2004). The main action applied to the manipulated variable *F* is on/off. This bang-bang action is determined using the estimated events ***e'***. Basically the "Events Software Sensor" (ESS) generates two types of ***e*** events estimation. A parameter $P \in (0,1)$ in Figure 1 tunes the points in μ where real ***e*** are located. Event ***e=a*** means that *S* is definitely above *S** and that μ is in the right-handed vicinity of point ***A***, i.e; moving away of the *P*-optimal zone. If the *F* pump is ON it must be turned OFF as shown in Figure 3. Similarly, ***e=b*** signals the moment in which the system is leaving the left border of the *P*-optimal zone, near point ***B***. If *F* pump is OFF then it must be switched ON as shown in Figure 3. The final reaction's time t_f will be close to the optimal t_{fopt} as the established on/off cycle will keep the system as close as desired to μ^* at all possible times, by properly choosing $P \to 1$ (Table 1).

The ESS is called this way because, without measuring the variables μ or *S* nor knowing the parameters *(S^*,μ^*)*, it estimates $e' \approx e$, using a real-time software algorithm. For doing so a γ variable must be available, such that its shape is related to the shape of μ, i.e. that as function of *S* its unique maximum coincides with *S**, regardless of other dependences it might have. For the case at hand γ is straightforwardly found in the gaseous product y:

$$\text{From (3):} \qquad \gamma \stackrel{\Delta}{=} y(S, X) = k_2 \mu(S) X \tag{6}$$

It is evident from (6) that for a given unknown X>0 and any unknown k_2>0 the shape of γ is the same as μ in Figure 1. That is, they grow monotonically from S=0 to $S=S^*$, and then they decrease, also monotonically, from $S=S^*$ and beyond as $S \to \infty$

But γ from (6) is useless as, except the fact they are positive, there is no available data for neither *S*, *X* nor k_2. That is why the ESS uses the time format of γ in (3) as it can be measured online and its maximum is easily found at some special times. Let's define t_k^* as the time when S just touches S^* for the k_{th} time. Then $\gamma_k^*=\gamma(t_k^*)$ is a detectable maximum. Later an k_{th} estimated event $\boldsymbol{e_k}$**'** will be provided at time t_{ek} when $\gamma(t_{ek})=P\gamma_k^*$ indicating that the system is about to leave the P-optimal zone. Note that this algorithm works independently of the structure or form of μ in (5), as long as it has a unique global maximum.

It should be noted in (3) that, as $X(t)$ may change with time, a slight difference in the t_{ek} is expected compared to the situation if μ were used directly instead of γ. This estimation inaccuracy decreases when $X(t)$ varies slower than $\mu(t)$. Three cases of interest might arise. In the first, the influent pump is OFF and S decreases. It might happen that γ is increasing which means that the system is inhibited and above or in the vicinity of S^* (see left-side of Figure 3). Instead, if γ decreases, this means that the system is below S^*. The second case takes place when the pump is ON and sufficient substrate is being added to the tank as to increase S at some rate. Here, if γ is increasing, it means the system is "below" or in the vicinity of S^*. On the opposite, if γ decreases, this means that there is substrate inhibition, above S^*. The third case should be avoided. It is the limit case where S_i in F is not sufficient to guarantee that the increase in S will produce a μ with a dynamics faster than that of X. This condition is easily avoidable, even if S_i changes over time, if the inflow provides significantly more substrate than would F_{opt}, the inflow needed for the optimal case (Moreno, 1999).

Figure 3 compares the behavior of the ED-TOC for two different values of P: P=P1=0.92 corresponds to the Figure 1. The second case P=P2=0.998 provides a much better efficiency at the detriment of the switching cycle for F. Table 1 summarizes the results for different values of P. There it can be seen that the switching time is reasonable for this application and that it can be enlarged, if necessary, accepting a small loss in optimality.

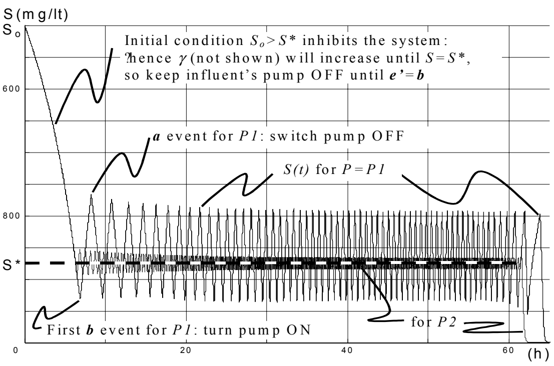

Figure 3. ED-TOC's Substrate kinetics for P1=0,92 and P2=0,998 shown together for comparison

Table 1 : ED-TOC optimality for different P

P	Optimality index t_{fopt}/t_f [%]	F pump cycles	Switching time [h]
0,998	99,9	448	0,14
0,98	99,8	151	0,41
0,96	99,2	106	0,59
0,90	96,0	62	1,0

4. ADAPTIVE EXTREMUM SEEKING

4.1. Principle and assumptions

The extremum-seeking scheme investigated here utilizes explicit structure information of the specific growth rate μ. In the case of Haldane kinetics (5) μ is maximum when the substrate concentrations equal to $S^*=\sqrt{K_S\cdot K_I}$. Then, the control objective is to keep the substrate concentration inside the reactor at the level S^*. Since the exact values of Haldane parameters are usually unknown (or at least poorly known), the adaptive extremum-seeking controller is developed to search this unknown set point such that the biomass production at the end of the reactor is maximized.

The adaptive extremum-seeking control scheme provides an adaptive control law of the dilution rate D to control the substrate S at the desired set point S^*, coupled with parameter learning laws for the Haldane model parameters. This algorithm requires the on-line knowledge of the substrate S and the gaseous outflow rate y (e.g. CO_2), as well as the related yield coefficients.

Parameter definition. Let's define:

$$\theta_\mu=\frac{\mu_0}{K_S},\ \theta_S=\frac{1}{K_S},\ \theta_I=\frac{1}{K_S\cdot K_I} \tag{7}$$

$\theta=\left[\theta_\mu\ \ \theta_S\ \ \theta_\mathrm{I}\right]^T$ represents the new set of kinetic parameters to be estimated on-line. The optimum for S can be re-expressed as follows: $S^*=\dfrac{1}{\sqrt{\theta_I}}$.

By this transformation, the optimum value is function of only one unknown parameter that has to be estimated on-line.

4.2. Estimation and Controller Design

The controller design proceeds in different steps. First, the estimation equation for S is derived from the balance model equation, then the control law and the estimation of the unknown kinetic parameters are included in a Lyapunov based derivation framework.

Estimation equation for the gaseous outflow rate y

By considering Eq. 1-3 and the kinetic parameter definition, the predicted state y is generated by:

$$\frac{d\hat{y}}{dt}=\frac{1-\hat{\theta}_i\,S^2}{S(1+\hat{\theta}_S\,S+\hat{\theta}_i\,S^2)}\left[D(S_i-S)-\theta_k y\right]y+ \\ +\frac{\hat{\theta}_\mu\,Sy}{1+\hat{\theta}_S\,S+\hat{\theta}_i\,S^2}-Dy+k_y e_y \tag{8}$$

with $k_y>0$ and $e_y=y-\hat{y}$. $\theta_k=\dfrac{k_1}{k_2}$ is the ratio of the yield coefficients, assumed to be known.

Design of the adaptive extremum-seeking controller

Since the parameter θ_I is unknown, the desired set point (x) can be re-expressed as follows: $S^* = \dfrac{1}{\sqrt{\hat{\theta}_I}}$.

The controller is designed in order to drive the substrate concentration *S* to the estimated value of *S** (x). An excitation signal *d(t)* is designed and injected into the adaptive system such that the estimated parameter $\hat{\theta}_I$ converges to its true value. The extremum seeking control objective can be achieved when the substrate concentration *S* is stabilized at the optimal operating set point *S**.

Define the error control variable z_S as follows:

$$z_S = S - \frac{1}{\sqrt{\hat{\theta}_I}} - d(t) \tag{9}$$

Consider the Lyapunov candidate function as follows:

$$V = \frac{z_S^2}{2} + \frac{1}{2}\cdot\left(\frac{\tilde{\theta}_\mu^2}{\gamma_\mu} + \frac{\tilde{\theta}_S^2}{\gamma_S} + \frac{\tilde{\theta}_I^2}{\gamma_I}\right) + \frac{e_y^2}{2}(1+\theta_S\cdot S+\theta_I\cdot S^2) \tag{10}$$

where $\tilde{\theta}_\mu = \theta_\mu - \hat{\theta}_\mu$, $\tilde{\theta}_s = \theta_s - \hat{\theta}_s$ and $\tilde{\theta}_I = \theta_I - \hat{\theta}_I$, γ_μ, γ_s and γ_I are positive tuning parameters.

The adaptive extremum seeking controller algorithm is derived from the expression of the Lyapunov candidate function V, in such a way that $\dot{V}$ is negative.

After mathematical manipulations, we obtain the control law and the parameter learning laws as follows:

Control law:

$$D = \frac{1}{S_i - S}\left[-k_Z z_S + \theta_k y + a(t) - k_d d(t)\right] \tag{11}$$

Note that the resulting control law consists of two terms: the first one includes the specific rates of the biomass growth, while the second is a correcting term proportional to the error output and to the dither signal, *d(t)* defined as:

$$\dot{d}(t) = a(t) + \frac{1}{2}\cdot\hat{\theta}_I^{-\frac{3}{2}}\cdot\frac{d\hat{\theta}_I}{dt} - k_d\cdot d(t) \tag{12}$$

where $a(t)$ acts as a dither signal on the closed-loop process and k_d is a strictly positive constant.

Parameter learning laws

$$\frac{d\hat{\theta}_\mu}{dt} = \gamma_\mu e_y S y \tag{13}$$

$$\frac{d\hat{\theta}_S}{dt} = \begin{cases} \gamma_S(\Gamma_1 D + \Gamma_2), \\ \quad \text{if } \theta_S > \varepsilon_s \text{ or } \theta_S > \varepsilon_s \text{ and } (\Gamma_1 D + \Gamma_2) > 0 \\ 0, \text{ otherwise} \end{cases} \tag{14}$$

$$\frac{d\hat{\theta}_i}{dt} = \begin{cases} \gamma_i(\Gamma_3 D + \Gamma_4), \text{ if } \theta_i > \varepsilon_i \text{ or } \theta_i > \varepsilon_i \\ \qquad \text{and } (\Gamma_3 D + \Gamma_4) > 0 \\ 0, \text{ otherwise} \end{cases} \tag{15}$$

where,

$$\Gamma_1 = -\frac{e_y(1-\hat{\theta}_i S^2)(S_i - S)y}{1+\hat{\theta}_S S + \hat{\theta}_i S^2} \tag{16}$$

$$\Gamma_2 = \frac{e_y(1-\hat{\theta}_i S^2)\theta_k y^2}{1+\hat{\theta}_S S + \hat{\theta}_i S^2} - \frac{e_y \hat{\theta}_\mu S^2 y}{1+\hat{\theta}_S S + \hat{\theta}_i S^2} \tag{17}$$

$$\Gamma_3 = -e_y S(S_i - S)y + \Gamma_1 \tag{18}$$

$$\Gamma_4 = e_y S\theta_k y^2 + S\,\Gamma_2 \tag{19}$$

and with the initial condition $\hat{\theta}_S(0) \geq \varepsilon_S = \dfrac{1}{K_{S,\max}} > 0$,

and $\hat{\theta}_i(0) \geq \varepsilon_i = \dfrac{1}{K_{S,\max}K_{I,\max}} > 0$.

The update laws are projection algorithms that ensures that $\hat{\theta}_S \geq \varepsilon_S > 0$ and $\hat{\theta}_i \geq \varepsilon_i > 0$.

By using appropriate mathematical arguments (that invoke in particular LaSalle invariance principle and Barbalat's lemma), it has been shown that if the dither signal fulfils some excitation persistence condition then the parameter estimates converges to their true values and the control error z_S converges to zero (Titica et al., 2003; Marcos et al., 2004).

5. SIMULATION RESULTS

The ED-TOC and the AES where tested using Matlab simulations, under different scenarios, for the same discontinuous reactor model. Each scenario in Table 2 provides a different challenge to the controllers.
The default kinetic model parameters and yield coefficients used to simulate the plant are:

$\mu_0 = 0.53h^{-1}, K_S = 1.2g/L, K_I = 0.22g/L$
$k_1 = 0.4, k_2 = 1.0$

The initial states, unless otherwise explicitly said, used during numerical simulations are:
$S_o = 2.0g/L, X_o = 7.2g/L, V_o = 1.0L$

and the substrate concentration in the inflow is $S_i = 20g/L$.

The optimality parameter for the ED-TOC controller was set to *P*=0.98 to calculate results in Table 3.

The design parameters for the AES controller were set to:
$\gamma_\mu = 10, \gamma_S = 200, \gamma_I = 200, k_{y,0} = 20, k_z = 0.5, k_d = 1,$
$\varepsilon = 0.2$. The dither signal *a(t)* is chosen as:

$$a = \sum_{i=1}^{5} A_{1i} \sin[(0.001 + (5 - 0.001)i/4)t] + \\ + \sum_{i=1}^{5} A_{2i} \cos[(0.001 + (5 - 0.001)i/4)t] \quad (20)$$

where A_{1i} and A_{2i} are normally distributed random numbers in the interval [-0.1, 0.1]. For details about the selection of the dither signal, the reader is referred to (Titica, et al., 2003).

The control objective is to fill the tank and obtain an amount of biomass, equal to that produced by the optimal trajectory, in the smallest possible time. The final reaction time t_f has been defined as the instant when $V(t_f)=V_{max}$=40L and $S_f=S(t_f)$<0.01 g/L, where this last value has been arbitrarily assigned.

An optimality index is defined as t_{fopt}/t_f, where t_{fopt} is the optimal, theoretical minimal, finishing time. Table 2 presents the optimality index for each case. It shows that the performance of both controllers is good and close to 100%, except in Scenarios 2 and 6. In Scenario 2 bad initial conditions for the kinetic parameters are given and, additionally, in Scenario 6 a sudden change in plant's kinetics is produced. In both cases the AES performs in a less optimal way because it requires some convergence time to adapt the estimated values of the true parameters of the plant, and meanwhile the AES uses a non-optimal set point. As long as the total change in S^* is not big enough to cause big efficiency loses, the performance will not be greatly affected. This is the case if some history about the plant's behavior exists, so the initial conditions for every new batch can be given in a trustable fashion. By comparison, the performance effect in the ED-TOC is almost negligible, if any. This is so because its operational principle is of the bang-bang type, meaning that at every instant in time it will do the best possible action to get the system in the P-optimal zone, without the need for allowing any parameter to converge. So the time the system spends away of the defined P-optimal zone depends only on the actuator limits and the plant dynamics. No equilibrium or set points are searched for. Its only aim is to keep the controlled variable inside the P-optimal zone during the singular arc. These are the main philosophical differences in both approaches. Table 3 shows another characteristics that define the main practical differences of the two controllers.

Some complementary differences between the two methods suggest some work should be done to combine them. In the AES, information about the plant is generated, as the values of the kinetic parameters are estimated in time. More sensors are used thus generating more data, specially S data. Other than the dither signal, it does not produce cycling of the input. On the other hand the ED-TOC is immune to tuning problems and model uncertainties (Table 3). It performs the bang-bang arcs in an exact way, same as the theoretical optimal solution. While doing the arcs it may know the t_k* instants when $S=S^*$ but does not know $S(t_k^*)$.

Figures 4 and 5 show the simulation results for Scenario 6. In Figure 4 it is clear that the dither in F, produced by the ED-TOC, is only plant-dependent, and that its convergence to new operation conditions is not governed by any controller's dynamics. The amplitude and time cycle of the bang-bang control signal depends only on the plant, and during the bang-bang arcs it operates perfectly. On the other hand, the AES graciously adjust its estimated value for the set-point of the manipulated variable (see dotted line in Figure 5), using an adaptive algorithm that requires a convergence time and that depends not only on the plants behavior in the new operational zone but also on the careful selection of the tuning parameters.

Table 2 : Optimality results for different scenarios for both controllers

Test Scenario for simulation comparison	Optimality index: t_{fopt}/t_f [%]	
	ED-TOC	AES
1. Default: $\mu o=0.53$ $Ki=0,22$ $Ks=1,2$ $(S^*=0,5138)$, True initial conditions given.	99.8	99.7
2. Bad initial kinetics given: μo=0.108 Ki=1,645 Ks=0,01 (S* decreased 50%)	99.8	89.5
3. Bad *So* given (increased 50% respect to the real value)	99.8	99.7
4. Measurement error of +20% for y in t=(20,30)	99.8	99.8
5. Measurement error of +20% for S in t= (20,30)	99.8	99.8
6. $So=S^*$, bad initial conditions given (S^* increased 100%), and S^* changed for $t=(20,50)$: $\mu o=0.53$ $Ki=0,44$ $Ks=2,4$ (S^* increased 100%)	99.1	96.5

Table 3 : Characteristic differentiation of both control philosophies

Characteristics	ED-TOC	AES
Measured variables:	y (used as γ)	S, y
Controlled variables:	μ	S
Manipulated variables:	F	D
Tuning parameters:	-	$\gamma_\mu, \gamma_S, \gamma_i, k_z, k_{y,0}, k_d, \varepsilon, a$
Optimality parameters:	P	-
Initial conditions required:	-	$S(0), y(0), S_f, \theta_\mu(0), \theta_S(0), \theta_i(0)$
Convergence speed depends on:	Plant and actuator limitations only	Plant and control tuning parameters
Control type:	Hybrid (Bang-bang + continuous)	Continuous

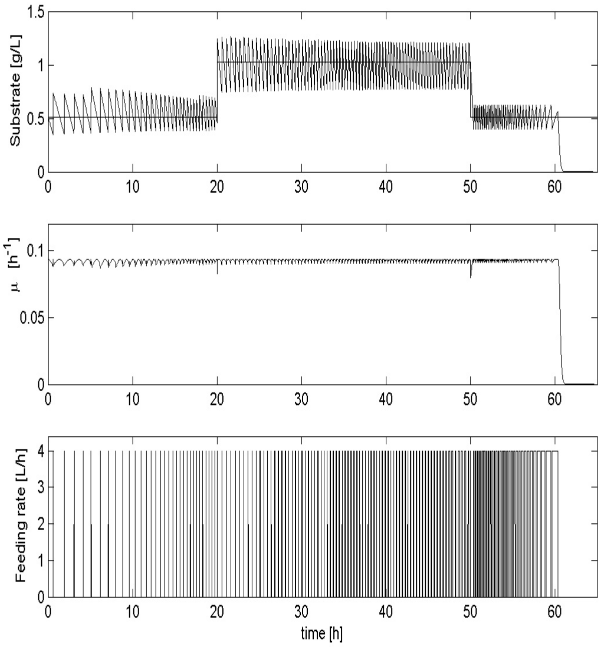

Figure 4: ED-TOC behavior using P=0.98 for Scenario 6 in Table 2. In the substrate plot S^* is drawn with a step-like line.

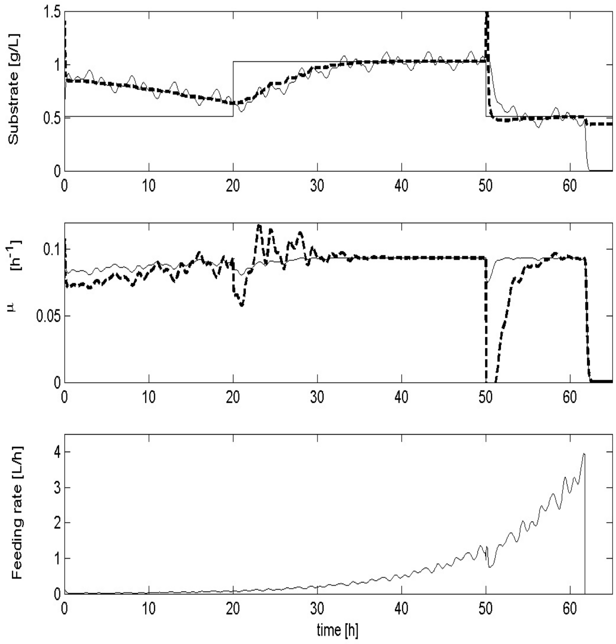

Figure 5: AES behavior for Scenario 6 in Table 2. In the substrate plot a step-like line shows S^*. Estimations are drawn with dashed lines.

6. CONCLUSIONS

Two control approaches of different philosophical nature have been compared, to understand their differences and complementarities, in a bioreactor example. The ED-TOC aims at keeping the system inside a predefined P-optimal zone. The AES aims at stabilizing the system in an optimal set point that is adapted on line. Both of them performed in a near optimal way for different test scenarios.

Advantages and disadvantages of the two philosophically different approaches were discussed, suggesting the possibility to combine them to obtain the better of each one of them. The idea is that while the system starts a batch, ED-TOC will performs in the best possible way for the singular arc. At the same time, if a S measure is available, during this bang-bang cycle a clear estimation of the P-optimal zone will be made in terms of S, including a measure for S^* at t_1^*. This value will be used to initialize the AES and, from then on, control could be made using AES policies. From time to time a bang-bang cycle could be run to test for optimality. This will reduce the on/off switching and at the same time bring valuable information about the plant model, and allow reacting to unforeseen perturbations or faults.

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Application of the event-driven time optimal control strategy for the degradation of inhibitory wastewater in a discontinuous bioreactor

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Keywords: optimal control, discontinuous process, SBR, 4-clorophenol, aerobic process, dissolved oxygen, respirometry, toxic wastewaters

Abstract: This work presents the results of the application of a new control strategy to optimize the degradation rate of toxic compounds. The event-driven time optimal control strategy (ED-TOC) was applied to biodegrade in a discontinuous reactor (SBR) a synthetic wastewater constituted with 4-chlorophenol (4CP) as model of the inhibitory compound. The ED-TOC strategy was developed in a manner to estimate a variable (named gamma) related to the substrate degradation rate in such a way that maximizing the former, the later is maximized too, but without measuring it. Gamma can be estimated in real time by using the dissolved oxygen concentration and the volume of the reactor. In the ED-TOC strategy, the influent flow rate is controlled in such a manner that the substrate degradation rate stays around its maximal value. To estimate gamma, only the mass transfer coefficient and the dissolved oxygen concentration at saturation are needed. It was found that a practical implementation of the ED-TOC strategy was possible. The degradation and mineralization of the 4CP were efficiently achieved. The average removal efficiencies were 99%, as chemical oxygen demand and 100% as 4CP. Total suspended solids at the effluent were below 14 mg/L, sludge volumetric index around 38 ml/g, and settling velocity of the sludge of 6 m/h. The ED-TOC strategy was able to manage increments of toxic concentrations in the influent up to 11200 mg 4CP/L. It was shown that not only higher concentrations of toxic could be treated with the ED-TOC strategy, but also a reduction in degradation time was obtained. For a given initial concentration of 4CP, the degradation rate was higher (almost doubled) with the ED-TOC strategy than the reaction rate obtained with the usual operation mode utilized in the SBR.

Introduction

The activated sludge process has been traditionally applied to treat industrial wastewater, but the nature of such discharges often causes operational problems in continuous flow systems. This is the case of the wastewaters containing toxic compounds generated by several chemical and petrochemical facilities. In such streams the mass of toxic contaminants varies with either time or space. Recently, innovative strategies like the discontinuous processes (controlled unsteady state processes) have been explored in order to increase the biotreatment efficiencies of wastewater (Buitrón *et al.* 2001). The term Sequencing Batch Reactor (SBR) is used as a synonym of the wastewater treatment technology where the volume of the reactor tank is variable in time (Wilderer *et al.* 2001). It can work with suspended or attached biomass. In general, the SBR process presented three major characteristics: periodic repetition of a sequence of well defined phases; planned duration of each process phase in accordance with the treatment result to be met and progress of the various biological and physical reactions as a function of time. Another characteristic of the SBR systems, because of their flexibility in control strategy, is that they are effective for fully automated computer controls.

Usually a SBR-type bioreactor operates under five well-defined phases: fill, react, settle, draw, and idle. The way in which the duration of each one of these phases is determined can be denominated operation mode and has a fundamental impact in the SBR characteristics. In the standard operation mode, the duration of these phases is typically determined by an expert operator based on his experience and exhaustive testing in the laboratory with a pilot plant. In particular, the reaction phase is sufficiently long to allow the toxic substances being degraded. The settle and draw phases are fixed in duration by the characteristics and constraints of the activated sludge and the reactor itself. Thus, this operational strategy could be considered as Fixed Timing Control strategy (FTC). Despite the inherent advantages of the discontinuous processes in relation to de biodegradation of toxic substances, the SBR operated under the FTC present several constraints when they are applied to the toxic wastewater degradation: inhibition of the microorganisms, problems with shock loads of toxic compounds, deacclimation and problems of starvation of the microorganisms and low efficiencies regarding the removal of toxic compounds (Buitrón and Moreno 2002; Buitrón et al, 2003).

To overcome the problems discussed above several operation modes have been presented using either dissolved oxygen (DO) concentration or the carbon dioxide evolution rate (CER) (Sheppard and Cooper, 1990; Buitrón *et al.* 1993; Nguyen *et al*., 2000). Moreno and Buitrón (1998) presented a methodology and mathematical simulations for the time optimal control of an activated sludge sequencing batch reactor (SBR) for toxic wastewater degradation. The optimal strategy for the input flow was obtained using techniques of optimal control theory, in which the reaction time is as small as possible. The degradation time was controlled through the substrate concentration estimated from the liquid oxygen concentration using an observer (Extended Kalman Filter). Vargas *et al*. (2000) presented the calibration of the observer and the experimental validation the Observer-Based Time Optimal Control strategy (OB-TOC). The drawback of this strategy is that it needs to know exactly the inflow substrate concentration and the constants of the Haldane model. This could make the OB-TOC difficult to apply in practice. Betancur *et al.,* (2004) described the mathematical development of a new Event-Driven Time Optimal Control strategy (ED-TOC) that measures the dissolved oxygen to robustly control the reaction rate of a discontinuous process treating inhibitory compounds.

This work presents the results of the application of the ED-TOC strategy to biodegrade, in a discontinuous reactor, a synthetic wastewater constituted with 4-chlorophenol as model of the inhibitory compound.

Methodology

Event-Driven Time Optimal Control Strategy

The ED-TOC strategy finds a variable (named γ) related to the reaction rate. Such variable can be estimated in real time by using the dissolved oxygen concentration and the volume of the reactor, as it was described in detail by Betancur *et al.* (2004). It is known that the behavior of the biomass growth rate (μ) as a function of the toxic substrate concentration (S) can be described by the Haldane law. In this model, μ reaches a maximal value, μ^*, when the substrate concentration is S^*. Toxic concentrations above or below μ^* will generate a diminution in the growth rate and, consequently, also in the reaction rate. Thus, if it is guaranty that S is near to S^*, it is also possible to maintain the degradation rate near to a maximal value. The problem consist, therefore, in to bring and to maintain μ at its maximal value during all the reaction period of the reactor. An additional problem is that μ is as much or more difficult to measure on-line in practice than the substrate concentration. It is interesting to point out that in the ED-TOC strategy it was developed a manner to estimate γ related to μ in such a way that maximizing the former, the later is maximized too, but without measuring it. In this case γ is proportional to μ by an unknown constant, which is not necessary to know for control purposes. Betancur *et al.* (2004) explained in detail how equation 5 was obtained from the model of a discontinuous reactor (equations 1 to 4):

$$\frac{dX}{dt} = \mu X - K_d X - X\frac{Q_{en}}{V} \qquad (1)$$

$$\frac{dS}{dt} = -\frac{1}{Y_{X/S}}\mu X + (S_{en} - S)\frac{Q_{en}}{V} \qquad (2)$$

$$\frac{dO}{dt} = -\frac{1}{Y_{X/O}}\mu X - bX + K_l a(O_s - O) + (O_{en} - O)\frac{Q_{en}}{V} \qquad (3)$$

$$\frac{dV}{dt} = Q \qquad (4)$$

$$\gamma = \frac{XV}{Y_{X/O}}\mu + bXV = K_l a(O_s - O)V - OQ_{en} + V\frac{dO}{dt} \qquad (5)$$

where,

X**:** Biomass concentration inside the reactor; ***S*****:** Substrate concentration inside the reactor; ***V*****:** Water volume level in the reactor; ***O*****:** Dissolved oxygen concentration, $\boldsymbol{Y_{X/S}}$**:** Biomass/substrate yield coefficient; $\boldsymbol{Y_{X/O}}$**:** Biomass/oxygen yield coefficient; $\boldsymbol{K_l a}$**:** Oxygen mass transfer coefficient; ***b*****:** Specific endogenous respiration rate; $\boldsymbol{K_d}$**:** Decay biomass rate; $\boldsymbol{\mu}$**:** Specific growth rate, $\boldsymbol{S_{en}}$**:** Influent substrate concentration; $\boldsymbol{O_{en}}$**:** Influent dissolved oxygen concentration; $\boldsymbol{Q_{en}}$**:** Influent flow rate; $\boldsymbol{O_s}$**:** Dissolved oxygen concentration at saturation; γ: variable proportional to $\boldsymbol{\mu}$.

Using the ED-TOC strategy, the influent flow rate is controlled in such a manner that the reaction rate stays inside the fast zone (gray zone in Figure 1). Such zone is above a P% of the maximum rate. The reaction rate is controlled maintaining the substrate concentration oscillating in a gap during the SBR filling. Every time the substrate concentration tries to leave this gap, an event is issued and the ED-TOC then switches the influent flow on/off, to prevent it. This will work regardless of the substrate influent concentration value and despite changes in most of the SBR parameters. All the variables in the right side of equation 5 are measurable or straightforwardly computable. Only the mass transfer coefficient, $K_l a$, and the dissolved oxygen concentration at saturation, O_s, are needed to estimate γ and they do not even need to be known precisely. This solution is therefore a good candidate for uses in real industrial environments.

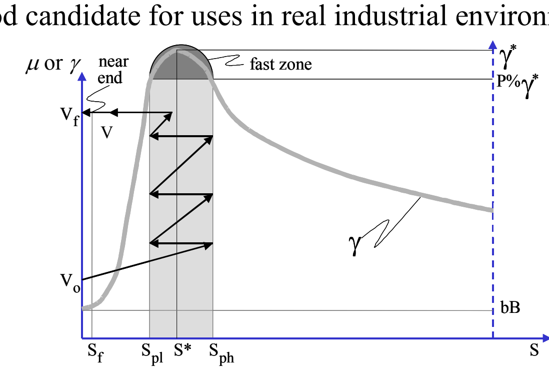

Figure 1 Plan trajectory for the ED-TOC strategy. Vo indicates the initial volume in the tank. The flow is feed to the reactor in such a manner to keep the reaction rate around the optimal value (gray zone). Once the final volume is reached, V_f, the reactor acts as a batch process and the reaction rate decreases.

Pilot reactor

An aerobic automated Sequencing Batch Reactor (SBR) system with a capacity of 7L and an exchange volume of 57% was used (Figure 2). The airflow rate was 1.5 liters per minute and the temperature was maintained at 20 ºC inside the reactor. The reactor was inoculated with microorganisms coming from a municipal activated sludge treatment plant (2000 mgVSS/L). A synthetic wastewater containing (4CP) was used as a sole source of carbon and energy. For standard conditions reactor was operated using an influent concentration of 350 mg 4CP/L. The strategy was tested using different initial concentrations of 4CP between 175 and 11200 mg/L, and also different airflow rates (0.75, 1.5 and 2.25 lpm). Nutrients such as nitrogen, phosphorus, and oligoelements were added following the techniques recommended by ANFOR (1985). The SBR was operated under the following strategy (except for acclimation period that is described above): preaeration time (15 min), filling and reaction time (variable depending on the influent concentration), settling time (30 min) and draw time (6 min).

Analytical methods

The substrate concentration was measured taking samples and processing them offline using the colorimetric technique of the 4-aminoantipyrine method (Standard Methods, 1992). Total and volatile suspended solids (TSS and VSS) analyses were determined according to the Standard Methods (1992). Dissolved organic carbon (DOC) was determined with a Shimadzu TOC-5050 and Chemical Oxygen Demand (COD) according to Standard Methods (1992). Theses analyses were performed to evaluate the 4CP mineralization. The metabolite (5-chloro-2hydroxy-muconic acid semialdehyde) (Commandeur and Parson, 1990), formed by an alternate degradation route of 4-CP by the microorganisms, and that can be inhibitory for the microorganisms, was also determined by spectrophotometry at 380 nm using a HACH spectrophotometer. Specific oxygen uptake rate (SOUR) experiments were conducted placing 10 mL of the mixed liquor of the SBR harvested just after a degradation cycle in a mini-reactor of 160 mL. An oxygen-saturated solution with nutrients and substrate (acetate or 4CP) was added and dissolved oxygen measured was recorded. Endogenous respiration was measured adding only nutrients. SOUR was computed from the slope of the reprogram divided by the VSS concentration.

Figure 2 Pilot reactor utilized for the toxic compounds degradation

Results and Discussion

Biomass Acclimation

The biomass was acclimated using a variable cycle strategy, i.e., the reaction phase duration was variable and stopped when the removal of 4CP was equal or greater than 95%. Acclimation was done using an initial 4CP concentration of 175 mg/L in the influent. When degradation time was constant, initial concentration was doubled and, then the reactor was maintained operating at 350 mg/L under the ED-TOC strategy. Figure 3 presents the evolution of the initial and final COD, as well as the TSS in the effluent. The average removal efficiency was 99%, as COD (483 and 5 mgDCO/L at influent and effluent, respectively) and 100% (as 4CP). Total suspended solids at the effluent were below 14 mg/L, sludge volumetric index around 38 ml/g, and settling velocity of the sludge of 6 m/h. These data indicate a good performance of the reactor operated with the ED-TOC strategy.

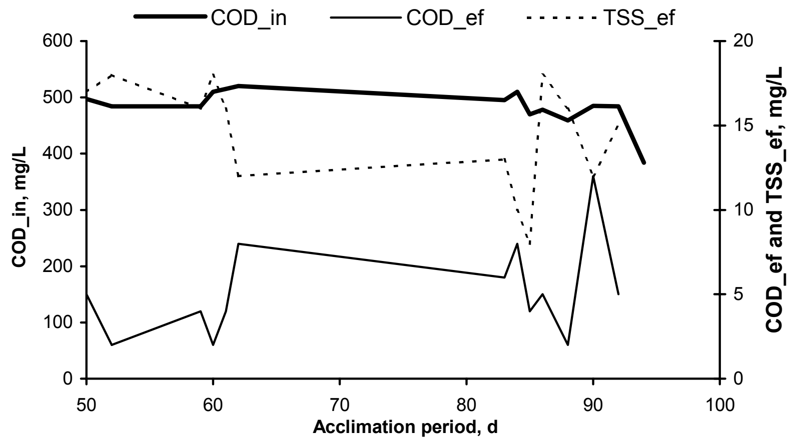

Figure 3 Evolution of the COD at the influent and effluent and TSS at the effluent for the process operated under the ED-TOC strategy.

Standard Conditions Kinetics

Figure 4 presents the behavior of the substrate concentration, measured as 4CP, COD, and DOC during a cycle operated under the ED-TOC strategy. It is possible to distinguish how the control operates following the substrate and the DO evolution curve. Once the influent begins to be fed to the reactor, the reaction starts. The DO decreases (first 0.2 h, figure 4) as the metabolic activity of the biomass increases to degrade the 4CP. Simultaneously, the estimator calculates γ and follow its value. When a maximal point is detected (before a minimum in the DO concentration), the feeding pump is turned off. In this point, the concentration of substrate is low than expected (it passed from 48 to 22 mg4CP/L, at 0.4 h in figure 4). Thus, the feeding pump is switched on, and a new charge of substrate is fed to the reactor. This procedure is repeated until the maximal volume has reached and then, the degradation proceeds in a batch manner. It is possible to observe in Figure 4 how the internal concentration of the reactor is maintained around 30 mg/L, which corresponds to a concentration close to S* and thus, around μ*. The metabolite production increases as the reaction took places, but after the cycle has finished, the metabolite concentration decreases, indicating a good operation of the system.

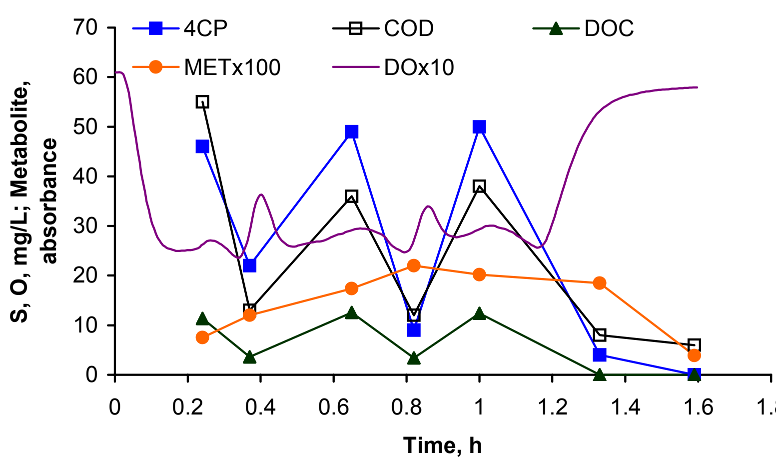

Figure 4 Evolution of the substrate concentration, measured as 4CP, COD, and DOC during a cycle operated under the ED-TOC strategy.

Performance of the ED-TOC strategy under different initial concentrations

In order to test the performance of the ED-TOC strategy in front of sudden incomes of concentration peaks to the plant, several initial concentrations of 4CP were tested. The performance of the reactor is compared to the response obtained by the reactor operated under the fixed timing strategy (FTC), a standard operation mode of the SBR. Table 2 summarized the results obtained. The reactor operated under the FTC strategy was able to manage concentration peaks up to 760 mg/L in the influent with an increment in the degradation time of 50%. In this case, it was necessary a week to recover the previous performance. Higher concentrations generated a severe problem of inhibition to the biomass. On the contrary, the ED-TOC strategy was able to manage increments of concentration in the influent up to 11200 mg/L. In theory, this strategy could treat any initial concentration in the tank. It is easy to demonstrate that not only higher concentration of toxic could be treated with the ED-TOC operation mode, but also a reduction in degradation time is obtained. If an initial concentration of 4CP of around 550 mg/L is considered, from table 1 it is observed that a specific degradation rates of 21 and 46 mg 4CP/gVSS –h are obtained for the FTC and the ED-TOC strategies, respectively. The degradation rate almost doubled with the optimal strategy for a same initial concentration of toxic to be treated.

Table 1. Effect of different operational strategies on the reactor performance under peaks of concentration.

Control strategy	Peak of 4CP, mg/L (S_{in})	Removal efficiencies during the peak (% of 4CP)	Degradation rate during the peak (mg 4CP/gVSS -h)	Performance of the reactor after the peak
FTC	550	100	21.0	No problem
FTC	760	85	18.5	Degradation time increases 50%. One week to recover previous performances
FTC	900	63	21.4	Severe affectation to the reactor performance. One month to recover.
ED-TOC	440	100	48.4	No problem
ED-TOC	530	100	45.8	No problem
ED-TOC	634	100	60.4	No problem
ED-TOC	700	100	63.5	No problem
ED-TOC	1400	100	91.2	No problem
ED-TOC	2800	100	114.3	No problem
ED-TOC	5600	100	114.3	No problem
ED-TOC	11200	100	114.3	No problem

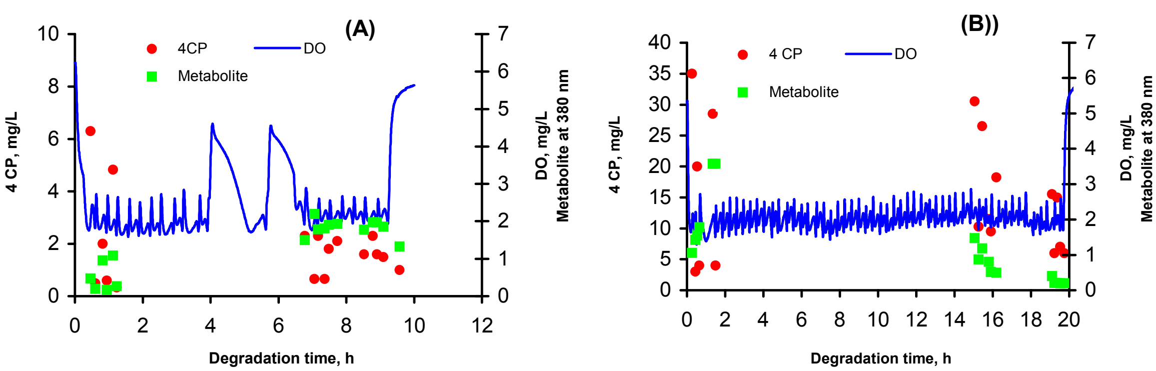

Figure 5 Degradation kinetics for an initial concentration of 2800 (A) and 5600 (B) mg 4CP/L using the ED-TOC strategy.

Dissolved Oxygen Variation

As the optimal strategy depends on the DO concentration to control the feed rate, it is important to study how much the variation in this parameter could affect the performance of the reactor. Two experiments were conducted varying the oxygen flow rate with respect to the standard value of 1.5 liters per minute. Figure 6 presents the evolution of the dissolved oxygen during the variation of ± 50 of the airflow in respect to standard conditions. For all the cases initial concentration of 4CP was 350 mg/L. When a –50% condition was applied, DO in the tank was always superior to 2 mg/L. Thus, it can be considered that no limitations for this element were present.

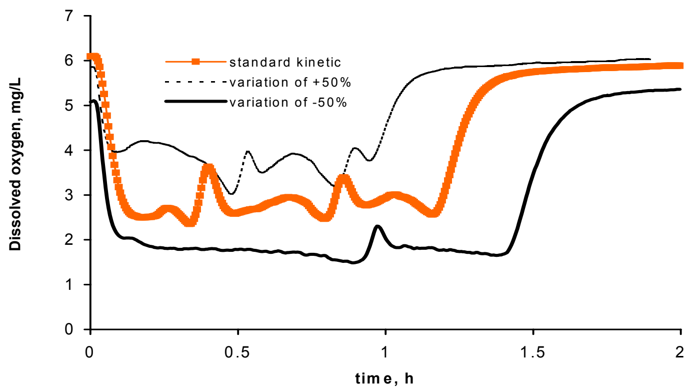

Figure 6 Evolution of the dissolved oxygen concentration as a function of time

Figure 7 shows the influence of the flow air variation on the substrate degradation (A) and on the metabolite production (B). In general, there was not a significant influence on the strategy operation when the air inflow rate was varied ± 50%. But, it is very interesting to note that in the case where the airflow was reduced by 50% there was an increase of the quantity of metabolite produced (Fig 7B). As a consequence, the degradation time for this same condition has a small increase (Fig 7A). Besides the influence on the metabolite production, this toxic by-product was no removed after the degradation cycle, which may cause problems due to the accumulation in the next cycles.

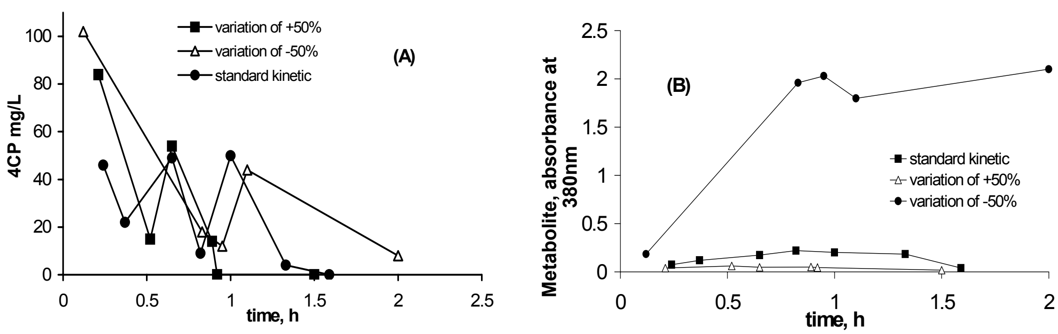

Figure 7 (A) Evolution during the degradation cycle of the 4CP concentration and the metabolite production (B) for different airflow rates

Conclusions

The application of a new control strategy to optimize the degradation rate of toxic compounds was presented. The event-driven time optimal control strategy (ED-TOC) was applied to biodegrade in a discontinuous reactor (SBR) a synthetic wastewater constituted with 4-chlorophenol (4CP) as model of the inhibitory compound. It was found that a practical implementation of the ED-TOC strategy was possible. A good performance of the reactor operated with the ED-TOC strategy was obtained since the degradation and mineralization of the 4CP was efficiently completed. The average removal efficiencies were 99%, as chemical oxygen demand and 100% as 4CP. Total suspended solids at the effluent were below 14 mg/L, sludge volumetric index around 38 ml/g, and settling velocity of the sludge of 6 m/h, which indicated the excellent settling characteristics of the sludge.

A better performance of the reactor operated with the ED-TOC strategy was observed when it was compared to the response obtained by the reactor operated under the fixed timing strategy. The ED-TOC strategy was able to manage increments of toxic concentrations in the influent up to 11200 mg 4CP/L without any problem. It was shown that not only higher concentrations of toxic could be treated with the ED-TOC strategy, but also a reduction in degradation time was obtained. For a given initial concentration of 4CP, the degradation rate was higher (almost doubled) with the ED-TOC strategy than the reaction rate obtained with the usual operation mode utilized in the SBR. In general, there was not a significant influence on the strategy operation when the air inflow rate was varied ± 50% in respect to the standard condition, but care must be taken when by-products are formed when aeration is not sufficient.

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BIODEGRADACIÓN DE EFLUENTES ALTAMENTE CONTAMINADOS POR COMPUESTOS FENÓLICOS UTILIZANDO UNA ESTRATEGIA DE CONTROL ÓPTIMA

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RESUMEN

El presente trabajo presenta los resultados del uso de una nueva estrategia del control para optimizar la tasa de degradación de compuestos tóxicos. La estrategia de control de tiempo óptimo por eventos dirigidos (ED-TOC) fue aplicada para biodegradar un agua residual sintética conteniendo 4-clorofenol (4CF) como compuesto inhibitorio modelo. Se utilizó un reactor discontinuo secuencial (SBR). La estrategia ED-TOC fue desarrollada para estimar una variable llamada gamma, relacionada con la tasa de la degradación del sustrato, de manera que la tasa de degradación sea la máxima. Se encontró que es posible la implementación práctica de la estrategia ED-TOC. El reactor presentó un buen funcionamiento ya que la mineralización del 4CF fue terminada eficientemente. Las eficiencias medias de remoción fueron del 99% como demanda química de oxígeno, y 100% como 4CF. Los sólidos suspendidos totales en el efluente se mantuvieron debajo de 14 mg/L, el índice volumétrico de lodos alrededor de 38 mL/g, y de la velocidad de sedimentación de 6 m/h, esto último indica que el lodo tuvo una excelente sedimentabilidad.

Palabras clave: SBR, control óptimo, proceso discontinuo, 4-clorofenol, oxígeno disuelto

INTRODUCCIÓN

El tratamiento de aguas por medio de lodos activados se ha aplicado tradicionalmente para tratar las aguas residuales industriales, pero la naturaleza de tales descargas causa a menudo problemas operacionales en sistemas de flujo continuos. Ésta es el caso de las aguas residuales que contienen compuestos tóxicos generados por industrias químicas y petroquímicas. En estos casos la cantidad de contaminantes tóxicos varía en tiempo y espacio.

Recientemente, las estrategias innovadoras como los procesos discontinuos se han explorado para aumentar las eficiencias del degradación de las aguas residuales (Buitrón *et al,.* 2001). El término SBR (reactor discontinuo secuencial por sus siglas en inglés) se ha utilizado como sinónimo de la tecnología del tratamiento de aguas residuales donde el volumen del tanque del reactor es variable en el tiempo (Wilderer *et al.,* 2001), estos reactores puede trabajar con la biomasa suspendida, fija o combinada en un lecho móvil. En general, los procesos en un SBR presentan tres características importantes: repetición periódica de una secuencia de fases bien definidas; la duración de cada fase del proceso puede ser determinada de acuerdo con el resultado de tratamiento que se espera y la realización de varias reacciones biológicas y físicas en función de tiempo. Por su flexibilidad, los sistemas SBR que pueden ser totalmente automatizados y controlados por una computadora.

Los sistemas de tipo SBR funcionan generalmente bajo cinco fases bien definidas: el llenado, reacción, sedimentación, vaciado, y tiempo muerto. En el modo de operación estándar, la duración de estas fases es determinada típicamente por un operador basado en su experiencia y en exhaustivas pruebas en el laboratorio con una planta experimental. En este modo de operación, la fase de reacción es suficientemente larga para permitir que las sustancias tóxicas sean degradadas. La duración de las fases de sedimentación y vaciado se fijan de acuerdo a las características del lodo activado y el reactor. Así, esta estrategia operacional se podría considerar como estrategia de tiempo fijo (FTC).

A pesar de las ventajas inherentes de los procesos discontinuos en lo referente a la biodegradación de sustancias tóxicas, un SBR que funciona bajo la estrategia de control FTC, tiene varios problemas cuando se emplea en la degradación de aguas residuales tóxicas: inhibición de los microorganismos, problemas con choques debido a un aumento repentino en la concentración del compuesto tóxico (picos de concentración), desaclimatación y problemas por ayuno de los microorganismos y bajas eficiencias en la remoción de compuestos tóxicos (Buitrón y Moreno 2004; Buitrón *et al.,* 2003).

Para superar los problemas discutidos sobre este modo de operación se han reportado el uso de la concentración de oxígeno disuelto (OD) o la tasa de variación del bióxido de carbono (Sheppard y Cooper, 1990; Buitrón *et al.*, 1993; Nguyen *et al.*, 2000). Moreno y Buitrón (1998) presentaron una metodología y simulaciones matemáticas para el control de tiempo óptimo de un SBR de lodos activados para la degradación de aguas residuales con compuestos tóxicos. La estrategia óptima para controlar el flujo de entrada fue obtenida usando las técnicas de la teoría de control óptimo, en las cuales el tiempo de reacción es tan pequeño como sea posible. El tiempo de la degradación es controlado con la concentración del sustrato estimada por medio de la concentración de oxígeno disuelto por medio del uso de un observador (filtro extendido de Kalman). Vargas *et al.* (2000) presentaron la calibración del observador y la validación experimental de la estrategia de tiempo óptimo basada en observadores. La desventaja de esta estrategia es que se necesita saber exactamente la concentración del sustrato en el flujo de entrada y las constantes del modelo de Haldane. Esto podría hacer que la estrategia sea difícil de aplicar en la práctica. Betancur *et al.,* (2004) describieron el desarrollo matemático de una nueva estrategia de control de tiempo óptimo por eventos dirigidos (Event-Driven Time Optimal Control, ED-TOC) la cual emplea la medición del OD para realizar el control de la degradación de compuestos inhibitorios por medio de un proceso discontinuo.

Este trabajo presenta los resultados del uso de la estrategia ED-TOC para biodegradar, en un reactor discontinuo, aguas residuales sintéticas constituidas con 4-clorofenol (4CF) como compuesto inhibitorio modelo

METODOLOGÍA

Estrategia de control de tiempo óptimo por eventos dirigidos (ED-TOC)

La estrategia ED-TOC estima una variable (llamada γ) relacionada con la tasa de reacción. Esta variable se puede estimar en tiempo real usando la concentración de oxígeno disuelto y el volumen del reactor, como fue descrito detalladamente por Betancur *et al.* (2004). A continuación se describe brevemente el método de estimación. Se sabe que para compuestos tóxicos el comportamiento de la tasa de crecimiento de la biomasa (μ), o la tasa de degradación de sustrato, en función de la concentración del substrato (S) se puede describir por la ley de Haldane. En este modelo, μ alcanza un valor máximo, μ*, cuando la concentración del substrato es S*. La concentración tóxica sobre o debajo de μ* generará una disminución en la tasa de crecimiento y, por lo tanto, también en la tasa de reacción. Así, si se garantiza que S está cerca a S*, la tasa de degradación estará cerca de un valor máximo.

El problema consiste, por lo tanto, encontrar y mantener μ en su valor máximo durante todo el período de reacción del reactor. Un problema adicional es que μ es muy difícil en la práctica medir en línea la concentración del sustrato. Es interesante precisar que en la estrategia de ED-TOC se desarrolló un método para estimar γ y relacionarla con μ de manera tal que ambos se encuentren en su valor máximo. En este caso γ es proporcional a μ por una constante desconocida, que no es necesaria saber para los propósitos del control.

La ecuación 5 fue obtenida del modelo de un reactor discontinuo (ecuaciones 1 a 4):

$$\frac{dX}{dt} = \mu X - K_d X - X\frac{Q_{en}}{V} \tag{1}$$

$$\frac{dS}{dt} = -\frac{1}{Y_{X/S}}\mu X + \left(S_{en} - S\right)\frac{Q_{en}}{V} \tag{2}$$

$$\frac{dO}{dt} = -\frac{1}{Y_{X/O}}\mu X - bX + K_l a\left(O_s - O\right) + \left(O_{en} - O\right)\frac{Q_{en}}{V} \tag{3}$$

$$\frac{dV}{dt} = Q \tag{4}$$

$$\gamma = \frac{XV}{Y_{X/O}}\mu + bXV = K_l a\left(O_s - O\right)V - OQ_{en} + V\frac{dO}{dt} \tag{5}$$

Donde:

X: Concentración de la biomasa dentro del reactor
S: Concentración del sustrato dentro del reactor
V: Volumen de agua dentro del reactor
O: Concentración de Oxígeno disuelto
$\boldsymbol{Y_{X/S}}$: Coeficiente de producción de Biomasa/sustrato
$\boldsymbol{Y_{X/O}}$: Coeficiente de producción Biomasa/oxígeno
$\boldsymbol{K_l a}$: Coeficiente de transferencia de masa
b: Tasa específica de respiración endógena

K_d: Tasa de decaimiento de la biomasa
μ: Tasa específica de crecimiento
S_{en}: Concentración de sustrato en el influente
O_{en}: Concentración de oxígeno disuelto en el influente
Q_{en}: tasa de flujo de entrada
O_s: Concentración de oxígeno disuelto a saturación
γ: variable proporcional a μ.

Usando la estrategia ED-TOC, el flujo de entrada es controlado de tal manera que la tasa de reacción permanezca dentro de la zona gris de la figura 1. Esta zona está en el punto donde la tasa de consumo de sustrato es la máxima. La tasa de reacción es controlada manteniendo la concentración del sustrato oscilando en este punto durante el llenado del SBR. Cada vez que la concentración del sustrato intenta dejar este punto, un evento es reportado y la estrategia ED-TOC enciende o apaga la bomba del flujo de entrada. La estrategia funciona a pesar de cambios de actividad de los microorganismos presentes en el SBR, tampoco importa el valor de la concentración de sustrato en el influente.

Todas las variables en el lado derecho de la ecuación 5 pueden ser medidas en forma directa. Para estimar γ solamente se necesita el coeficiente de transferencia de masa, K_la y la concentración de oxígeno disuelto a la saturación, O_s. Incluso, estas variables no necesitan ser conocidas con precisión. Esta solución es por lo tanto un buen candidato a aplicaciones en ambientes industriales verdaderos.

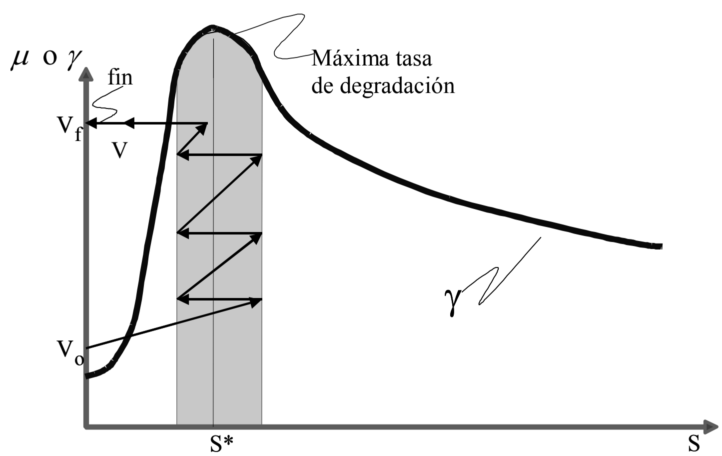

Figura 1. Estrategia ED-TOC. Vo indica el volumen inicial en el tanque. El flujo es alimentado de manera tal que se mantiene la tasa de reacción cerca del valor óptimo (zona gris) Una vez que se alcance el volumen final, Vf, el reactor actúa como un proceso en lotes (batch) y la tasa de reacción disminuye

Reactor piloto

Se empleó un reactor aerobio discontinuo secuencial con una capacidad de 7L y un volumen de intercambio de 57% (figura 2). El flujo de aire empleado fue de 1.5 litros por minuto y se mantuvo una temperatura de 20 °C dentro del reactor. El biorreactor fue inoculado con microorganismos provenientes de una planta de tratamiento de aguas residuales municipales (2000 mg SSV/L). Se empleo un agua sintética que contenía 4CF como única fuente de carbono y energía. Se agregaron nutrientes como nitrógeno, fósforo y oligoelementos siguiendo la recomendación de AFNOR (1985).

Para las condiciones consideradas como estándar, el reactor fue alimentado con una concentración en el influente de 350 mg4CF/L. Esto quiere decir que, tomando en cuenta el volumen intercambiado, dentro del reactor la concentración inicial fue de 200 mg4CF/L. Se evaluaron diversas concentraciones iniciales de 4CF entre 175 y 11200 mg/L para probar la estrategia de control, y también diversos flujos de aire (0.75, 1.5 y 2.25 litros por minuto). La duración de las fases del SBR fue la siguiente: tiempo de preaeración (15 minutos), llenando y reacción (variable, dependiendo de la concentración del influente), sedimentación (30 minutos) y vaciado (6 minutos).

Figura 2. Reactor piloto usado en la degradación de compuestos tóxicos

Métodos analíticos

La concentración del sustrato fue medida tomando muestras y procesándolas fuera de línea por medio de la técnica colorimétrica de la 4-aminoantipirina (Standard Methods, 1992). Los análisis de sólidos suspendidos totales y volátiles (SST y SSV) fueron determinados de acuerdo a Standard Methods (1992). El carbono orgánico disuelto (COD) fue determinado con por medio del sistema Shimadzu TOC-5050 y la demanda química de oxígeno (DQO) según Standard Methods (1992). Estos análisis fueron realizados para evaluar la mineralización del 4CF.

El metabolito (5-cloro-2hidroxi- ácido semialdehido mucónico) (Commandeur y Parson, 1990), es formado por una ruta alterna de la degradación de 4-CF por los microorganismos, y es inhibitorio para los microorganismos, fue determinado por espectrofotometría a 380 nm usando un espectrofotómetro HACH.

Se realizaron experimentos para conocer la tasa específica de consumo de oxígeno (TECO), por medio de un mini reactor de 160 ml donde se colocaban 10 mL del licor mezclado del SBR obtenido después de un ciclo de degradación. Se agregó una solución saturada de oxígeno con nutrientes y sustrato (acetato o 4CF) y la medición del oxígeno disuelto fue registrada. La respiración endógena fue medida agregando solamente nutrientes. La TECO fue obtenida de la pendiente de consumo de oxígeno dividida entre la concentración de SSV.

RESULTADOS Y DISCUSIÓN

Aclimatación de la biomasa

La biomasa fue aclimatada por medio de la estrategia de tiempos variables, en la cual la duración de la fase de reacción fue detenida cuando la remoción del 4CF fuera igual o mayor a 95%. La aclimatación se realizó usando una concentración inicial 4CF de 175 mg/L en el influente. Cuando el tiempo de la degradación fue constante, la concentración inicial fue aumentada al doble, es decir, el reactor era mantenido degradando 350 mg/L de 4CF bajo estrategia ED-TOC. La figura 3 presenta la variación de la DQO inicial y final, así como los SST en el efluente.

La eficiencia promedio de remoción fue del 99% como DQO (483 y 5 mgDQO/L en el influente y el efluente, respectivamente) y 100% (como 4CF). Los sólidos suspendidos totales en el efluente fueron menores a 14 mg/L, de índice volumétrico de lodos se mantuvo alrededor de 38 mL/g y la velocidad de sedimentación del lodo de 6 m/h. Estos datos indican un buen funcionamiento del reactor operado con la estrategia de control ED-TOC.

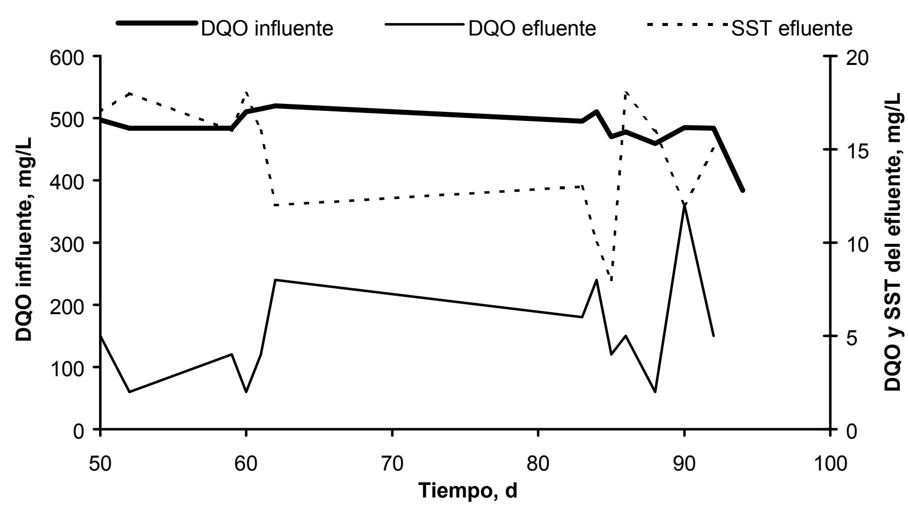

Figura 3. Variación de la DQO en el influente y efluente, y SST en el efluente del proceso operado bajo la estrategia de control ED-TOC

Cinéticas de la condición estándar

La figura 4 presenta el comportamiento de la concentración de sustrato, medido como 4CF, DQO y COD durante un ciclo operado bajo estrategia de control ED-TOC. Es posible distinguir como funciona la estrategia de control siguiendo los cambios en la curva de degradación del sustrato y el OD. En esta estrategia el reactor comienza operando como Fed-batch. Una vez que el sustrato comienza a ser alimentado al reactor, la reacción comienza. El OD disminuye (primeras 0.2 h, figura 4) como resultado del aumento en el consumo de oxígeno debido al aumento en la actividad metabólica de la biomasa para degradar el 4CF. Simultáneamente, el estimador calcula γ y monitorea este valor. Cuando se detecta el punto máximo de γ (antes de que exista una concentración mínima de OD), la bomba de alimentación se apaga. Después de que la concentración de sustrato disminuye (de 48 a 22 mg4CF/L, en 0.4 h en la figura 4) el sistema detecta que la concentración del sustrato se vuelve menor a la esperada para obtener una γ máxima (es decir, ya no es la óptima), por lo cual también se observa que la actividad de los microorganismos comienza a dejar de ser la máxima. Así, el sistema enciende la bomba de alimentación, y una nueva carga de sustrato se alimenta al reactor. Se repite este procedimiento hasta que se alcanza el volumen máximo del reactor y con lo cual la degradación continua como un proceso batch clásico.

Es posible observar en la figura 4 cómo la concentración dentro del reactor se mantiene alrededor de 30 mg/L durante la alimentación dosificada hecha por el sistema de control, esta concentración de sustrato corresponde a una concentración cercana a S* y por lo tanto alrededor de μ*. La producción del metabolito se incrementa cuando la reacción se lleva a cabo, pero después de que el ciclo ha terminado, la concentración del metabolito disminuye, indicando una buena operación del sistema.

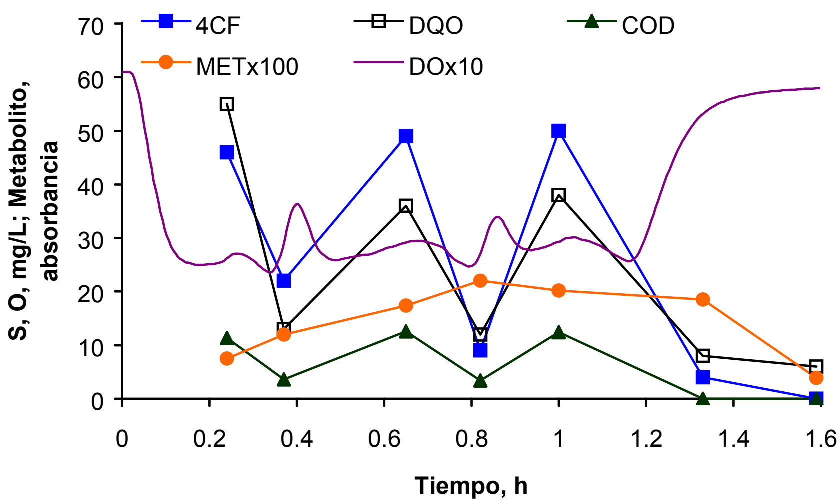

Figura 4. Variación de la concentración del sustrato, medido como 4CF, DQO y COD durante el ciclo operado con la estrategia ED-TOC

Funcionamiento de la estrategia ED-TOC bajo diferentes concentraciones iniciales

Para probar el funcionamiento de la estrategia de ED-TOC bajo picos de concentración (exposición repentina a altas concentraciones de tóxico), se evaluaron varias concentraciones iniciales de 4CF. Se comparó la respuesta obtenida con la estrategia ED-TOC y la obtenida cuando el reactor operó con una estrategia de tiempo fijos (FTC). La tabla 1 resume los resultados obtenidos. El reactor que funcionó bajo la estrategia FTC pudo degradar picos de concentración de hasta 760 mg4CF/L en el influente con un incremento en el tiempo de degradación del 50%. En este caso, fue necesaria una semana para recuperar el buen funcionamiento del reactor y la actividad inicial de los microorganismos. Concentraciones más altas de 4CF generaron un problema severo de inhibición a la biomasa del cual el reactor no se recuperó.

En caso contrario, la estrategia ED-TOC pudo manejar incrementos de la concentración en el influente de hasta 11200 mg4CF/L. En teoría, esta estrategia podría tratar cualquier concentración inicial en el tanque. Es fácil demostrar que no sólo una concentración más alta de compuesto tóxico se podría tratar con la estrategia de operación ED-TOC, sino que también es obtenida una reducción en tiempo de degradación. En las figuras 5 y 6 se presentan las cinéticas de degradación de 4CF y el OD durante la degradación de 2800 y 5600 mg4CF/L con la estrategia ED-TOC.

Considerando una concentración inicial de 550 mg/L, se obtuvieron tasas específicas de degradación de 21 y 46 mg 4CF/gSSV-h, para la estrategia FTC y la estrategia ED-TOC, respectivamente (tabla 1). La tasa de degradación fue casi del doble con la estrategia EDTOC para una misma concentración inicial de tóxico tratado.

Tabla 1. Efecto de diferentes estrategias de operación sobre el desempeño de un reactor bajo la exposición a picos de concentración

Estrategia de control	Pico de 4CF, mg/L (S_{in})	Eficiencia de remoción durante el pico (% of 4CF)	Tasa de degradación durante el pico (mg 4CF/gSSV-h)	Desarrollo del reactor después del pico
FTC	550	100	21.0	No hay problemas
FTC	760	85	18.5	Incremento del tiempo de degradación en un 50%. Fue necesaria una semana para recuperar la eficiencia original
FTC	900	63	21.4	Afectación severa sobre el desempeño del reactor. Fue necesario un mes para recobrar la eficiencia original
ED-TOC	440	100	48.4	No hay problemas
ED-TOC	530	100	45.8	No hay problemas
ED-TOC	634	100	60.4	No hay problemas
ED-TOC	700	100	63.5	No hay problemas
ED-TOC	1400	100	91.2	No hay problemas
ED-TOC	2800	100	114.3	No hay problemas
ED-TOC	5600	100	114.3	No hay problemas
ED-TOC	11200	100	114.3	No hay problemas

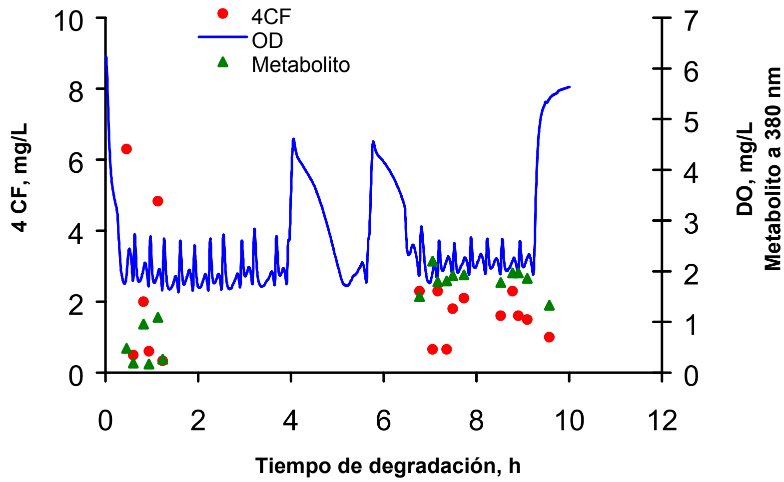

Figura 5. Cinética de degradación para una concentración inicial de 2800 mg4CF/L usando la estrategia ED-TOC

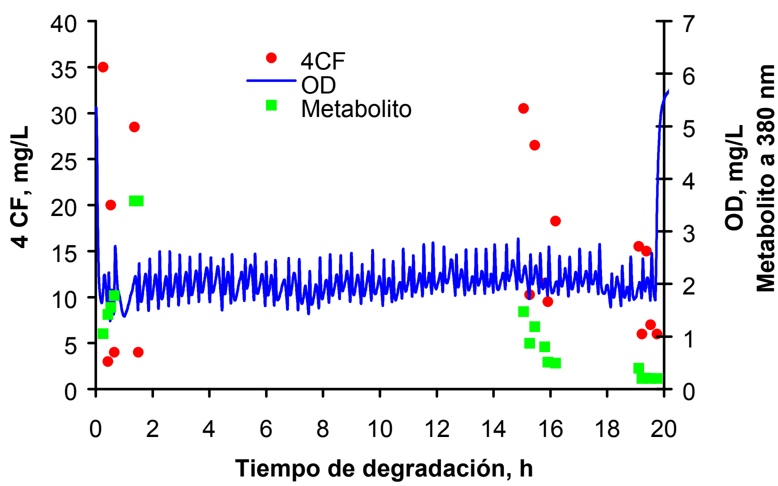

Figura 6. Cinética de degradación para una concentración inicial de 5600 mg4CF/L usando la estrategia ED-TOC

Variación del oxígeno disuelto

Ya que la estrategia de tiempo óptimo depende del OD para controlar el flujo de alimentación de sustrato, es importante estudiar cuánto podría afectar la variación de este parámetro en el funcionamiento del reactor. Se realizaron dos experimentos variando el flujo del aire con respecto al valor estándar de 1.5 litros por minuto. La figura 7 presenta la evolución del oxígeno disuelto durante la variación de ± 50 del flujo de aire en referencia a la condición estándar. Para todos los casos la concentración inicial de 4CF fue 350 mg/L. Cuando una condición de -50% fue aplicada, el OD en el reactor siempre fue superior a 2 mg/L. Con lo cual se puede considerar que no hubo limitaciones para este elemento en el reactor y que la estrategia puede operar bien aún en condiciones no óptimas.

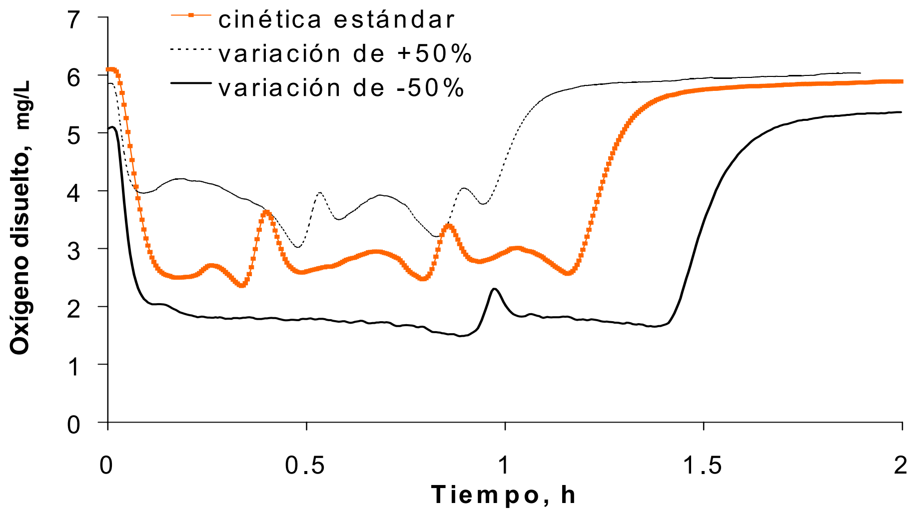

Figura 7. Variación de la concentración de oxígeno disuelto en función del tiempo

La figura 8 muestra la influencia de la variación del flujo del aire en la degradación del substrato (A) y en la producción del metabolito (B). En general, no hubo una influencia significativa en la operación de la estrategia cuando la tasa de flujo de aire varió en un ±50%. Pero, es muy interesante observar que en el caso donde el flujo de aire fue reducido 50% hubo un aumento de la cantidad de metabolito producido (figura 8B). Por consiguiente, el tiempo de degradación para esta misma condición aumenta (figura 8A). Además de la influencia en la producción del metabolito, este subproducto tóxico no fue removido en el ciclo de degradación, lo cual puede causar problemas debido a la acumulación en los ciclos siguientes.

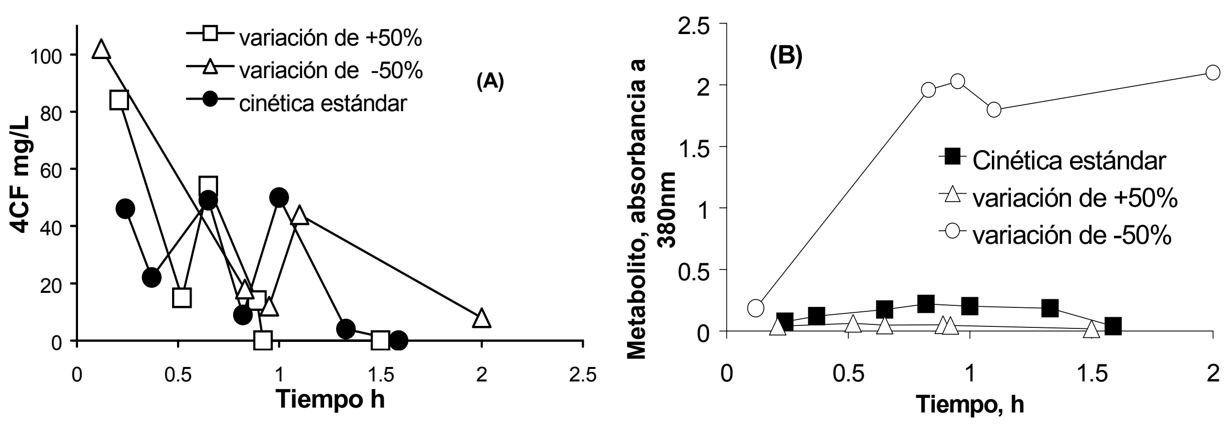

Figura 7. (A) Degradación del 4CF en diferentes concentraciones iniciales de 4CF y la producción de metabolito (B) para diferentes flujos de aire

CONCLUSIONES

Se demostró la factibilidad de la aplicación de una nueva estrategia del control para optimizar la tasa de degradación de compuestos tóxicos. La estrategia de control de tiempo óptimo por eventos dirigidos (ED-TOC) fue aplicada para biodegradar 4-clorofenol (4CF) como compuesto inhibitorio modelo en un reactor discontinuo secuencial (SBR). El reactor presentó un buen funcionamiento ya que la mineralización del 4CF fue terminada de manera eficiente. Las eficiencias medias del remoción fueron del 99% como demanda química de oxígeno, y 100% como 4CF. Los sólidos suspendidos totales en el efluente se mantuvieron debajo de 14 mg/L, el índice volumétrico de lodos alrededor de 38 mL/g, y de la velocidad de sedimentación de 6 m/h, esto último indica que el lodo tuvo una excelente sedimentabilidad.

Al operar el reactor con la estrategia ED-TOC se observó un excelente funcionamiento, superior al mostrado por la estrategia de tiempos fijos (FTC). La estrategia de ED-TOC puede manejar incrementos en la concentración de compuestos tóxicos en los influentes de 11200 mg4CF/L sin ningún problema. Fue demostrado que no sólo concentraciones más altas de tóxico se podrían tratar con la estrategia de ED-TOC, sino que también se obtuvo una reducción en tiempo de degradación. Para una concentración inicial dada de 4CF, la tasa de degradación fue más alta (casi el doble) con la estrategia de ED-TOC que con la estrategia FTC. En general, no hubo una influencia significativa en la operación de la estrategia ED-TOC cuando el flujo de aire se varió en ±50% con respecto a la condición estándar, pero se debe tener cuidado con los subproductos (metabolito) ya que se incrementaron cuando la aireación no fue suficiente

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GLOBAL OBSERVABILITY AND DETECTABILITY ANALYSIS OF UNCERTAIN REACTION SYSTEMS

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Abstract: Observation issues for reaction systems is of fundamental importance since there is a lack of sensors and the uncertainties can be very high. The objective of this work is to propose a methodology to make a global analysis of observability and detectability of such systems, with a particular concern about the design of unknown input observers.

Keywords: Observability, indistinguishability, detectability, uncertain reaction systems, Unknown input observer

1. INTRODUCTION

Reaction systems is a class of nonlinear dynamical systems that is widely used in areas such as chemical and biochemical engineering, biomedical engineering, biotechnology, ecology, etc. (Robust) Observation issues for this class of systems is of fundamental importance since there is a lack of sensors and the uncertainties can be very high. It is not surprising that there is a intensive research activity to design observers, or software sensors, for these systems (Bastin and Dochain, 1990; Dochain and Vanrolleghem, 2001; Dochain, 2003). It is well known, that the existence of observers for dynamical systems is intrinsically related to the observability, or detectability, of the system. However, there are few studies in the literature dealing with the observability, detectability properties of reacting systems. Most of these studies are local in nature (Dochain and Chen, 1992). However, a satisfactory solution to the observation problem is global, since it seems unreasonably to require that the initial condition of the system is up to a small error known, when one of the motivations to use an observer is precisely the lack of information on this initial state!

The objective of this work is to propose a methodology to make a global analysis of observability and detectability of reaction systems. This is in contrast to the usual local results of the literature. When there are no uncertainties the usual method to do a global observability analysis is by means of the observability map (Zeitz, 1989; Gauthier and Kupka, 2001). However, there is no systematic method to study detectability for nonlinear systems. In this work a methodology is presented to carry out a *global* observability/detectability analysis of *uncertain* reaction systems, when the uncertainty is represented as an arbitrary and unknown input signal. For this kind of systems

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no method is known to study observability. This method is an extension for the uncertain case of the idea used for the analysis of the induction machine under sensorless operation (Ibarra-Rojas *et al.*, 2004). Other approaches are given in (Ponzoni *et al.*, 2004), based on structural information, but restricted to non dynamical representations of the plant in steady state. The cornerstone of this result is the *strongly indistinguishable trajectories* concept (internal trajectories of a system that are different under the same input/output behavior under uncertain inputs) and the main result is the *characterization* of *the complete set* of this kind of functions for the uncertain reaction system, including both types of indistinguishable trajectories: the divergent (non-observable) ones, i.e. those which are not possible to identify by input/output measurements, and the asymptotically convergent (detectable) ones, i.e. those that can be determined by the input/output behavior asymptotically. The proposed methodology achieves the desired characterization by constructing a nonlinear dynamical system, called *strongly indistinguishable dynamics*, whose set of solution trajectories corresponds to the aforementioned set of strongly indistinguishable behaviors, i.e. every solution trajectory of this system is an strongly indistinguishable trajectory for the studied system. We shall be able to give some sufficient conditions for an uncertain reaction system to be observable/detectable or to be not observable/not detectable.

The paper is organized as follows. A general model of reaction systems is given in Section 2. Global observability/detectability properties are introduced for uncertain systems and their relationship with the existence of observers is studied in Section 3. In Sections 4 and 5 the observability properties of uncertain reaction systems is analyzed and their consequences for observer design is given in Section 6.

2. MODEL OF REACTION SYSTEMS

A general state-space model of reaction systems is generally obtained from mass and energy balances (Bastin and Dochain, 1990; Dochain *et al.*, 1992; Dochain and Vanrolleghem, 2001) :

$$\frac{dc}{dt} = \bar{K}\varphi(c,T) + D(c_{in} - c) - Q_c(c,T) + \bar{F}$$
$$\frac{dT}{dt} = -\frac{1}{\rho C_p}\Delta H^T \varphi(c,T) + D(T_{in} - T) - Q_T$$

where $c \in \mathbb{R}^{n-1}$, $T \in \mathbb{R}$, $\bar{K} \in \mathbb{R}^{(n-1)\times q}$, $\varphi \in \mathbb{R}^q$, $D \in \mathbb{R}$, $Q_c \in \mathbb{R}^{n-1}$, $\bar{F} \in \mathbb{R}^{n-1}$, $\rho \in \mathbb{R}$, $C_p \in \mathbb{R}$, $\Delta H \in \mathbb{R}^q$, $Q_T \in \mathbb{R}$, $c_{in} \in \mathbb{R}^{n-1}$ and $T_{in} \in \mathbb{R}$ are the component concentration vector, the temperature, the stoichiometric coefficient matrix, the reaction rate vector, the dilution rate, the gaseous outflow rate vector, the feedrate vector, the density, the heat capacity, the reaction heat vector, the heat exchange term, and the inlet concentration vector and temperature, respectively. In most applications the measured variables are a subset of the state variables or, more generally, a linear combination of them.

This system can be written in a compact and generalized form as

$$\Sigma_R : \begin{cases} \dot{x} = K\varphi(x) + D(x_{in} - x) - Q(x) + F \ , \\ y = Cx \ . \end{cases} \tag{1}$$

where $x \in \mathbb{R}^n$ is the state, and $y \in \mathbb{R}^m$ is the output vector. This model includes also the case when several reactors are considered, for which $D \in \mathbb{R}^{n\times n}$ is a matrix. In practice the knowledge of the model is usually very uncertain, since the parameters and nonlinearities of the system are difficult to identify, and they change over the time. In particular, the reaction rates are usually poorly known. This makes the observation problem challenging. In this paper we will concentrate on the case when the reaction rates are unknown, but the rest of the model is assumed to be known, i.e. $u = F - Q(x) + Dx_{in}$ is considered a known signal (Bastin and Dochain, 1990). This uncertainty will be modelled as an (arbitrary) unknown input $w = \varphi(x)$.

3. OBSERVABILITY AND DETECTABILITY CONCEPTS FOR NONLINEAR UNCERTAIN SYSTEMS AND EXISTENCE OF OBSERVERS

Since the uncertainties in the reaction system (1) will be represented by unknown inputs, let us consider a general nonlinear system described by

$$\Sigma : \begin{cases} \dot{x} = f(x,u,w) \ , \quad x(0) = x_0 \\ y = h(x) \ , \end{cases} \tag{2}$$

where $x \in \mathbb{R}^n$ is the state vector, $u \in \mathbb{R}^p$ is the input vector, $w \in \mathbb{R}^q$ is a vector of unknown inputs, $y \in \mathbb{R}^m$ is the output vector, and f and h are sufficiently smooth functions. The solution of (2) passing through x_0 at $t = 0$ and corresponding to the input function $u(\cdot)$, and $w(\cdot)$, is denoted as $x(t, x_0, u(\cdot), w(\cdot))$. In a similar way, let us denote the output $y(t, x_0, u(\cdot), w(\cdot)) = h(x(t, x_0, u(\cdot), w(\cdot)))$. Whenever there is no confusion, these will be simply denoted as $x(t)$ and $y(t)$. Let us assume in addition that the system Σ is *complete*, i.e. the state trajectories $x(t)$ are defined for every $t \geq 0$, every initial condition $x_0 \in \mathbb{R}^n$ and every input $u(\cdot) \in \mathcal{U}$, and $w(\cdot) \in \mathcal{W}$, classes of input functions.

For systems without unknown inputs a basic concept is that of indistinguishable states (Hermann and Krener, 1977). Roughly speaking two states are said to be indistinguishable if they are different although both the input and the output of the system are identical. The importance of this definition comes from the fact that observer's existence for the system strongly relies on the existence (and the type) of this kind of functions. For systems with unknown inputs (2) similar concepts can be introduced.

Definition 1. (**Strong Indistinguishability, and Observability and Strong(*) Detectability**) Consider for system (2) an input $u(\cdot)$, an initial condition $x \in \mathbb{R}^n$ and an unknown input $w(\cdot)$. If $\bar{x} \in \mathbb{R}^n$, $\bar{x} \neq x$, is such that $y(t, x, u(\cdot), 0) = y(t, \bar{x}, u(\cdot), w(\cdot))$, for all $t \in [0, \infty)$, and for some $w(\cdot) \in \mathcal{W}$, then $\bar{x}$ is a *strongly* $u(\cdot)$-*indistinguishable* state of x. The set of all strongly $u(\cdot)$-indistinguishable states of x will be denoted by $\mathcal{I}^{UI}_{(u,x)}$.
System (2) is *strongly observable* if for every $x \in \mathbb{R}^n$, and every $u(\cdot) \in \mathcal{U}$ $\mathcal{I}^{UI}_{(u,x)} = \{x\}$.
System (2) is *strongly detectable* if for every $x \in \mathbb{R}^n$, every $u(\cdot) \in \mathcal{U}$, and for every $\bar{x} \in \mathcal{I}^{UI}_{(u,x)}$ and the corresponding $w(\cdot)$ that renders $\bar{x}$ indistinguishable $\lim_{t\to\infty} \|x(t, \bar{x}, u(t), w(\cdot)) - x(t, x, u(t), 0)\| = 0$.

System (2) is *strong* detectable* if for some $x, \bar{x} \in \mathbb{R}^n$, $u(\cdot) \in \mathcal{U}$ and $w(\cdot) \in \mathcal{W}$ it happens that $\lim_{t\to\infty} \|y(t, \bar{x}, u(t), w(t)) - y(t, x, u(t), 0)\| = 0$,then it follows that $\lim_{t\to\infty} \|x(t, \bar{x}, u(t), w(t)) - x(t, x, u(t), 0)\| = 0$.

Note that strong detectability excludes the existence of diverging strongly indistinguishable trajectories. It may be surprising that two detectability definitions have been introduced. For LTI systems without unknown inputs it is well-known that if the inobservable subsystem is asymptotically stable then if as $t \to \infty$ $y(t) \to 0$ then $x(t) \to 0$. However, for continuous time systems with unknown inputs this is not longer the case, as has been pointed out by (Hautus, 1983).

Remark 2. It is clear that strong* detectability implies strong detectability, but the converse is not true. Moreover, strong observability implies strong detectability, but it does not necessarily imply strong* detectability.

These properties are indeed related to the existence of Unknown Input Observers (UIO).

Definition 3. **(UI Observer)** Consider a system

$$\Omega : \begin{cases} \dot{z} = \varphi(z, u, y) \ , & z(0) = z_0 \\ \hat{x} = \chi(z, u, y) \ , & \end{cases} \tag{3}$$

where $z \in \mathbb{R}^r$ is the state vector and φ, χ are functions defined in $(z, u, y) \in \mathbb{R}^r \times \mathbb{R}^p \times \mathbb{R}^m$. $z(t, z_0, u, y)$ denotes a solution of (3) passing through z_0 at $t = 0$ and corresponding to u and y.
System (3) is called an *unknown input observer (UIO)* for system (2) if $\exists z_0 \in \mathbb{R}^r$ such that $\forall x_0 \in \mathbb{R}^n$, $\forall u(\cdot) \in \mathcal{U}$ and $\forall w(\cdot) \in \mathcal{W}$

$$\lim_{t\to\infty} \|\hat{x}(t, z_0, u, y(t, x_0, u, w)) - x(t, x_0, u, w)\| = 0 \ .$$

Note that in this definition no major restriction has been imposed on the observer, except for the convergence of the observer for *every* trajectory, i.e. initial condition and input, of the plant.

For LTI systems it is shown by (Hautus, 1983) that strong* detectability is equivalent to the existence of an UIO, and that strong detectability or observability are not sufficient for the existence of an UIO. Let us now partially generalize the concept for nonlinear systems.

The following result is indeed valid for every reasonable definition of observer, since it depends on a structural restriction of the system and not on the structure of the observer.

Lemma 4. If system (2) has an unknown input global observer, then it is strong* detectable. Moreover, if the convergence of the observer can be assigned arbitrarily fast, then it is strongly observable.

PROOF. Suppose that system (2) is not strong* detectable. Then there exist an input $u(\cdot)$, two states $x_1, x_2 \in \mathbb{R}^n$, and an unknown input $w(\cdot)$ such that as $t \to \infty$, $y(t, x_1, u, 0) \to y(t, x_2, u, w)$, but $x(t, x_1, u, 0) - x(t, x_2, u, w) \nrightarrow 0$. For an UI (global) observer Ω of Σ there exists $z_0 \in \mathbb{R}^r$ such that $\hat{x}(t, z_0, u, y(t, x_1, u, 0)) \to x(t, x_1, u, 0)$, and $\hat{x}(t, z_0, u, y(t, x_2, u, w)) \to x(t, x_2, u, w)$. Note that

$\hat{x}(t, z_0, u, y(t, x_1, u, 0)) \to \hat{x}(t, z_0, u, y(t, x_2, u, w))$.
But since

$$\begin{aligned} &\lim_{t\to\infty} \{x(t, x_1, u, 0) - x(t, x_2, u, w)\} = \\ &\quad = \lim_{t\to\infty} \{x(t, x_1, u, 0) - \hat{x}(t, z_0, u, y_1)\} + \\ &\quad + \lim_{t\to\infty} \{x(t, x_2, u, w) - \hat{x}(t, z_0, u, y_2)\} = 0 \ , \end{aligned}$$

the assumption on x_1, x_2 is contradicted.
To prove the second assertion, suppose by contradiction, that there are two convergent indistinguishable trajectories. Then an observer cannot converge to the correct state at a rate greater than the convergence rate of the trajectories. □

From this lemma it is clear that for studying the possibility of estimating or not state trajectories of a given dynamical system, one can first investigate the existence of robust indistinguishable trajectories, and then determine if they are converging or not, i.e. if the system is robust detectable or observable.

4. THE ERROR AND INDISTINGUISHABLE DYNAMICS OF REACTION SYSTEMS

The conditions given above are abstract and no checkable conditions were given. The objective of this section is to introduce a dynamical interpretation of the concepts introduced in the previous section. This interpretation will be used in the following section to derive necessary conditions for the existence of global observers. This dynamic characterization, although possible for a general nonlinear system, will be derived here for the case of interest in the paper, the uncertain reaction system (1). It will be assumed that the model is well-known, except for the reaction rates that are completely unknown, so that they can be considered as unknown inputs.

The following Gedanken-experiment leads to the desired characterization of strong* and strong detectability: Two identical systems, but with different initial conditions and unknown inputs, evolve in time

$$\begin{aligned} \dot{x}_i &= Kw_i - Dx_i + u \ , \ x_i(0) = x_{i0} \ , \\ y_i &= Cx_i \ , \qquad i = 1, 2 \ . \end{aligned}$$

Introducing the variables $x = x_1$, $y = y_1$, $w = w_1$, and $\tilde{x} = x_1 - x_2$, $\tilde{y} = y_1 - y_2$, $\tilde{w} = w_1 - w_2$, the error dynamics of the plant is given as

$$\begin{aligned} \dot{x} &= Kw - Dx + u \ , \ x(0) = x_0 \ , \\ \dot{\tilde{x}} &= K\tilde{w} - D\tilde{x} \ , \ \tilde{x}(0) = \tilde{x}_0 \ , \\ y &= Cx \ , \\ \tilde{y} &= C\tilde{x} \ . \end{aligned} \tag{4}$$

Since for this system the evolution of x does not affect the error state $\tilde{x}$, the basic properties can be studied via the reduced linear system

$$\begin{aligned} \dot{\tilde{x}} &= -D\tilde{x} + K\tilde{w} \ , \ \tilde{x}(0) = \tilde{x}_0 \ , \\ \tilde{y} &= C\tilde{x} \ . \end{aligned} \tag{5}$$

Consider also the linear Differential-Algebraic (DA) system,

$$\begin{aligned} \dot{\tilde{x}} &= -D\tilde{x} + K\tilde{w} \ , \ \tilde{x}(0) = \tilde{x}_0 \ , \\ 0 &= C\tilde{x} \ . \end{aligned} \tag{6}$$

derived from (5) by setting $\tilde{y}(t) = 0$ for all $t \geq 0$. This system will be called the (reduced) *Strongly Indistinguishable Dynamics* of the plant (1) with unknown reaction rates. Strong(*) detectability and observability of the plant can be determined and characterized analyzing the properties of the solution set of the Strong Indistinguishable Dynamics. The following result is a simple consequence of the definitions.

Lemma 5. Consider the system (1), with unknown reaction rates.

(1) Two trajectories are *strongly indistinguishable* if and only if they are of the form $x(t, x_0, u(t), w(\cdot))$, and $x(t, x_0, u(t), w(\cdot)) + \tilde{x}(t, \tilde{x}_0, \tilde{w}(\cdot))$, where $x(t)$ is a solution of (1) and $\tilde{x}(t)$ is a solution of (6).
(2) The system is *strongly detectable* if and only if the constrained system (6) is globally asymptotically stable.
(3) The system is *strongly observable* if and only if the constrained system (6) is trivial, i.e. the only solution is $\tilde{x}(t) = 0$.
(4) The system is *strong* detectable* if and only if for the system (5) whenever $\lim_{t\to\infty} \tilde{y}(t) = 0$ it follows that $\lim_{t\to\infty} \tilde{x}(t) = 0$.

In the special case considered in this paper, the indistinguishable dynamics (5) is very simple, since it is decoupled from the plant, and because it is a linear time-varying system. This allows a very deep analysis, that is seldom possible.

Recall that a usual characterization of the zeros (or zero dynamics) of a system corresponds to the set of pairs of initial conditions and inputs, such that the output of the system is zero for all the time. This means that the *zero dynamics* of the indistinguishable dynamics (5) is given by the constrained system (6). Note that the strong indistinguishable trajectories correspond to the trajectories of the zero dynamics, that strong observability is equivalent to the absence of strong indistinguishable trajectories, i.e to the absence of zeros, and strong detectability coincides with the asymptotic stability of the zero dynamics.

Lemma 5 gives a dynamical interpretation of the observability/detectability concepts for the specific case considered. It is clear, that this idea can be used for more general systems, although the obtained indistinguishability dynamics systems are, in general, not so simple as here. Compared to the usual observability criteria, that are based on constructing the observability map with the vector fields, this characterization has several advantages. 1) The approach is not local whether in time nor in the state space. 2) It allows to determine detectability, what is usually impossible in the other criteria. 3) The dynamical interpretation is appealing. 4) Several nonlinear tools can be used to make the analysis, as for example the characterization of the zero dynamics in geometric control. 5) Lyapunov functions can be used for the characterization of the properties. 6) It is of very general nature. No special smoothness or structural properties are necessary. 7) For systems with unknown inputs there is no observability test based on the system vector fields in the literature.

5. DETECTABILITY ANALYSIS FOR UNCERTAIN REACTION SYSTEMS

The analysis of the error dynamics (4) provides basic information for the design of UIO's. Since strong* detectability is a necessary condition for the existence of UIO (see Lemma 4), the objective is to determine conditions on the system, such that when $\tilde{y} \to 0$ as $t \to \infty$ it follows that $\tilde{x} \to 0$ as $t \to \infty$. Since D is in general a time varying matrix the results for the LTI case of (Hautus, 1983) do not apply. It is clear that asymptotic stability of the zero dynamics (6), i.e. *asymptotic minimum phaseness*, or equivalently strongly detectability, is a necessary property. Sufficient conditions (in the LTI case also necessary) are:

Proposition 6. Consider the system (5) with constant matrices C and K, and a uniformly bounded time-varying matrix D. $\tilde{y} \to 0$ as $t \to \infty$ implies $\tilde{x} \to 0$ as $t \to \infty$ if

(1) $\operatorname{rank}(CK) = \operatorname{rank}(K)$,
(2) System (5) is exponentially minimum phase, i.e. the system described by the DAE (6) has an exponentially stable equilibrium point.

PROOF. Define a regular output transformation

$$\bar{y} = \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \end{bmatrix} = S\tilde{y} = \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} \tilde{y} \qquad (7)$$

where $S_1 \in \mathbb{R}^{q \times m}$, $S_2 \in \mathbb{R}^{(m-q)\times m}$, and S is regular. Due to condition (1) S_1, S_2 and M, such that $MK = 0$, can be so selected, that

$$T = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} = \begin{bmatrix} S_1 C \\ S_2 C \\ M \end{bmatrix},$$

defines a state transformation $z = T\tilde{x}$. Defining $z_i \triangleq T_i \tilde{x}$, $i = 1, 2, 3$, system (5) in the new coordinates is given by

$$\begin{aligned} \dot{z}_1 &= \bar{D}_{11} z_1 + \bar{D}_{12} z_2 + \bar{D}_{13} z_3 + w \\ \dot{z}_2 &= \bar{D}_{21} z_1 + \bar{D}_{22} z_2 + \bar{D}_{23} z_3 \\ \dot{z}_3 &= \bar{D}_{31} z_1 + \bar{D}_{32} z_2 + \bar{D}_{33} z_3 \\ \bar{y} &= \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \end{bmatrix} = \bar{C} z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \end{aligned} \qquad (8)$$

where

$$\bar{D} = -TDT^{-1} = \begin{bmatrix} \bar{D}_{11} & \bar{D}_{12} & \bar{D}_{13} \\ \bar{D}_{21} & \bar{D}_{22} & \bar{D}_{23} \\ \bar{D}_{31} & \bar{D}_{32} & \bar{D}_{33} \end{bmatrix},$$

$$\bar{C} = SCT^{-1} = \begin{bmatrix} I_q & 0 & 0 \\ 0 & I_{m-q} & 0 \end{bmatrix}.$$

The zero dynamics of the original system in the new coordinates is then

$$\dot{z}_3 = \bar{D}_{33} z_3 \ , \ 0 = \bar{D}_{13} z_3 + w \ , \ 0 = \bar{D}_{23} z_3 \qquad (9)$$

that by hypothesis is assumed to be exponentially stable. By standard results of input/output stability of LTV systems (Callier and Desoer, 1991) it follows that when $z_1 \to 0$, and $z_2 \to 0$ then $z_3 \to 0$ as $t \to \infty$ in system (8), and therefore $\tilde{y} \to 0$ implies $\tilde{x} \to 0$ for (5). □

Remark 7. Note that the first condition implies that $m \geq q$, i.e. the number of measurements has to be larger than the number of unknown inputs.

Remark 8. Exponential minimum phaseness has to be required, since for LTV systems asymptotic stability does not assure input/output stability (see (Rugh, 1993)), that is required in the subsystem z_3 in (8). To clarify this observation consider the scalar system with bounded coefficients

$$\begin{aligned} \dot{x}(t) &= \frac{-2t}{t^2+1} x(t) + u(t) \ , \ x(t_0) = x_0 \ , \\ y(t) &= x(t) \ . \end{aligned}$$

This system is not exponentially stable since the transition matrix is given by

$$\Phi(t, t_0) = \frac{t_0^2 + 1}{t^2 + 1} \ .$$

But it is uniformly stable, and the zero-input response goes to zero for every initial state. However, it is not BIBO stable and a vanishing input does not produce a vanishing output, i.e. $u \to 0 \not\Rightarrow y \to 0$ as $t \to \infty$. To see this consider the output response for $t_0 = 0$ and $x_0 = 0$

$$y(t) = \frac{1}{t^2+1} \int_0^t \left(\tau^2 + 1\right) u(\tau)\, d\tau \ .$$

With $u(t) = 1$ the output $y(t) = \left(t^3 + 3t\right)/3\left(t^2+1\right)$ is unbounded. For $u(t) = t^r/\left(t^2+1\right)$, with $1 < r < 2$, $u(t) \to 0$ but $y(t) = t^{(r+1)}/(r+1)\left(t^2+1\right)$ is unbounded! And so in general exponential stability has to be imposed. However, exponential minimum phaseness is also not necessary. Consider for example subsystem z_3 in (8), and that $\bar{D}_{31} = 0$, and $\bar{D}_{32} = 0$. In this case asymptotic minimum phaseness is sufficient to assure the convergence.

Remark 9. It is interesting to note, that it is possible to have a system that is strong* detectable and strongly observable. This is the case when the only solution of (9) is $z_3 = 0$. However, this is not possible if $m = q$.

6. OBSERVER DESIGN

For LTI systems the conditions in the previous proposition are also sufficient for the existence of an UIO. For time-varying systems this seems not to be the case. However, under some mild further assumptions (always satisfied in the LTI case), an UIO can be constructed. For simplicity it will be assumed that the plant has been transformed according to the state and output transformation introduced in the proof of Proposition 6.

Proposition 10. Consider the reactor system (1) with constant matrices C, and K, and a uniformly bounded time-varying matrix D, that satisfies the conditions of Proposition 6 and is represented in new coordinates as

$$\begin{aligned}
\dot{\xi}_1 &= \bar{D}_{11}\xi_1 + \bar{D}_{12}\xi_2 + \bar{D}_{13}\xi_3 + w + u_1 \\
\dot{\xi}_2 &= \bar{D}_{21}\xi_1 + \bar{D}_{22}\xi_2 + \bar{D}_{23}\xi_3 + u_2 \\
\dot{\xi}_3 &= \bar{D}_{31}\xi_1 + \bar{D}_{32}\xi_2 + \bar{D}_{33}\xi_3 + u_3 \\
\bar{y} &= \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \end{bmatrix} = \bar{C}\xi = \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} .
\end{aligned}$$

Consider the subsystem independent of the unknown input

$$\begin{aligned}
\dot{\xi}_2 &= \bar{D}_{21}\xi_1 + \bar{D}_{22}\xi_2 + \bar{D}_{23}\xi_3 + u_2 \\
\dot{\xi}_3 &= \bar{D}_{31}\xi_1 + \bar{D}_{32}\xi_2 + \bar{D}_{33}\xi_3 + u_3 \\
\bar{y}_2 &= [0, I, 0]\,\xi = \xi_2 ,
\end{aligned}$$

and a reduced order UIO for the plant of the form

$$\begin{aligned}
\dot{\hat{\xi}}_2 &= \bar{D}_{21}\bar{y}_1 + \bar{D}_{22}\hat{\xi}_2 + \bar{D}_{23}\hat{\xi}_3 + u_2 + L_1(\hat{y}_2 - y_2) \\
\dot{\hat{\xi}}_3 &= \bar{D}_{31}\bar{y}_1 + \bar{D}_{32}\hat{\xi}_2 + \bar{D}_{33}\hat{\xi}_3 + u_3 + L_2(\hat{y}_2 - y_2) \qquad (10) \\
\hat{y}_2 &= [0, I]\,\hat{\xi} = \hat{\xi}_2 ,
\end{aligned}$$

(1) If the pair $\left([I, 0], \begin{bmatrix} \bar{D}_{22} & \bar{D}_{23} \\ \bar{D}_{32} & \bar{D}_{33} \end{bmatrix}\right)$ is UCO, then (10) is a reduced order UI observer whose convergence dynamics can be arbitrarilly assigned.
(2) If the pair $\left([I, 0], \begin{bmatrix} \bar{D}_{22} & \bar{D}_{23} \\ \bar{D}_{32} & \bar{D}_{33} \end{bmatrix}\right)$ is uniformly detectable, then (10) is a reduced order UI observer.

It is interesting to note that the results derived in the literature under the name asymptotic observer (Bastin and Dochain, 1990), that are able to estimate the state of a bioreactor without knowledge of the reaction rates, are especial cases of the results in this paper. In fact, our results are a justification from the observability/detectability point of view of the asymptotic observers.

In particular if D is a scalar, i.e. $D = d\mathbb{I}$, then if the measurements are so selected, that condition (1) of Proposition 6 is satisfied, then condition (2) is equivalent to the persitence of excitation of the input $d(t)$ (Bastin and Dochain, 1990). In this case it is however impossible to satisfy condition (1) of Proposition 10, an so it is not possible to assign the convergence dynamics of the UIO, no matter how the measurements are selected.

7. CONCLUDING REMARKS

In this paper a new method has been proposed for the characterization of the observability/detectability properties of uncertain reaction systems, when the uncertainty is modelled as an arbitrary unknown input. A fairly complete characterization of these properties for the reactor system with unknown reaction rates has been obtained using this method, and sufficient conditions for the possibility of constructing robust (asymptotic) observers have been given. These initial results opens the possibility to study further other situations in a methodological manner. This will be pursued in future work.

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CONTROL STRATEGIES FOR TREATING TOXIC WASTEWATER USING BIOREACTORS

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Abstract: Different control strategies are compared, in regard to issues associated to biomass inhibition when treating toxic wastewater, to operate sequencing batch bioreactors. In particular the problem of time optimal operation and also the problem of handling sudden unknown toxicant peak concentrations are addressed. Because of the application characteristics it is not feasible, nowadays, to measure all of the important variables, thus little information is available online for controlling the process. One of the alternatives presented, the Event-Driven Time Optimal Control, offers to solve all problems, using only the practically available variables, even if uncertainties are present in the mathematical model of the bioreactor. *Copyright © 2004 IFAC*

Keywords: optimal control, *software sensor*, *fed-batch*, bioreactor, toxic wastewater.

1. INTRODUCTION

Biological treatment of highly toxic wastewater, as such produced by the chemical and petrochemical industries, is a difficult task. Sequencing batch reactors (SBR) have demonstrated their superiority for uses in wastewater treatment (WWT), compared to continuous reactors, mainly because of their performance. This paper shows how SBRs may be further enhanced with the use of suitable control strategies. In general traditional SBR processes exhibit 3 characteristics: periodical repetition of a defined phases sequence (filling, reaction, settling, draw and idle time) for each batch, dynamical behavior of biological and physical reactions in time and a preprogrammed duration of each phase according to the expected results, i.e. Fixed Timing Control (FTC). The first interesting SBR problem to solve is related to instrumentation limitations: it is not feasible, nowadays, to use toxicant substrate concentration ($\boldsymbol{S}$) measurements. Then, for the FTC strategy, an expert chooses the timing based on the expected values for the toxicant substrate concentration in the inflow ($\boldsymbol{S_i}$). However, if the given reaction time falls short, the SBR won't finish the substrate degradation and then toxicants will be dumped at the end of the batch. To be on the safe side, the reaction time is usually set bigger than necessary. This wastes time and potentially causes a second problem: if all toxicant substrate is quickly treated the biomass starves while waiting the next phase. Starvation may alter biomass necessary acclimation to such toxicant (Coello *et al.,* 2003; Buitrón and Moreno 2002). A third related problem is the lack of processing time optimality, i.e. toxicant treatment in minimum time. A fourth problem is model uncertainty, especially in the $\boldsymbol{S}$ nonlinear relation to μ, the biomass growth rate (see Fig.1). As substrate degradation rate is directly related to μ, it follows that the maximum degradation rate is attained when $\boldsymbol{S}=\boldsymbol{S}^*$, as only at

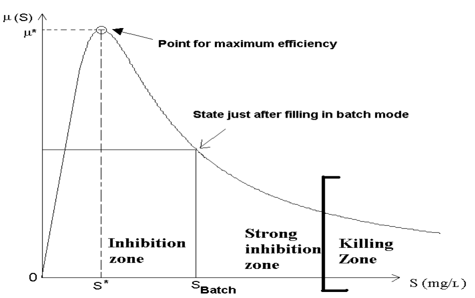

Figure 1. Biomass specific growth rate $\mu(S)$

this point μ reaches its global maximum μ*. But FTC does not take this into account. Filling is performed at the higher possible flow rate, i.e. pure batch mode, regardless of $\boldsymbol{S_i}$ value. Hence the maximum $\boldsymbol{S}$ value inside the reactor ($\boldsymbol{S_{Batch}}$) is only function of the unknown $\boldsymbol{S_i}$. As typically $\boldsymbol{S_{Batch}}$ is higher than $\boldsymbol{S}$* then "inhibited" is the, undesirable, normal status for the SBR (see Fig. 1) in FTC mode. A fifth potential problem, even worse, appears if a sudden unknown toxicant peak is fed to the SBR. Here $\boldsymbol{S_{Batch}}$ may go to the killing zone, endangering the SBR, i.e. permanently damaging the biomass.

The simplest way to improve FTC is to detect the end of the reaction phase, without measuring $\boldsymbol{S}$, by using the easy and cheap to measure Dissolved Oxygen concentration ($\boldsymbol{O}$) in a similar way as proposed in (Sheppard and Cooper, 1990). That is what the Variable Timing Control (VTC in Table 1) (Buitrón et al., 2003) does. In the past, optimal control theory has been used to tackle some of the SBR problems allowing finding the best feeding policy, i.e. fed-batch mode (Smets et al., 2002; Sarkar and Modak, 2003; Moreno, 1999), but it is usually necessary to know perfectly the model of the plant and to measure its whole state. These conditions are very restrictive: a perfect model and parameter knowledge is very often unrealistic and, in WWT, it is either impossible or very expensive to measure all state variables. Such Time Optimal Control (TOC), when influent pump actuator limits are considered, consists of 3 arcs. Fig. 2(b2) depicts, for SBR model in Eq. (1-4), the optimal trajectory projected in the Substrate-Volume plane (TP-SV): a *bang-bang* arc that fills the SBR until $\boldsymbol{S}$=$\boldsymbol{S}$*, a singular arc that controls the feeding to maintain $\boldsymbol{S}$=$\boldsymbol{S}$* (this is the vertical path of the TP-SV, meaning $\boldsymbol{S}$ does not change even if volume level $\boldsymbol{V}$ increases), and a final *bang-bang* arc that waits until $\boldsymbol{S}$ decays below some final $\boldsymbol{S_f}$. As $\boldsymbol{S}$ is not available, two strategies, close to that theoretical TOC are proposed: observer based time optimal control (OBTOC in Table 1) (Vargas et al., 2000) and event based time optimal control (EDTOC in Table 1) (Betancur *et al.*, 2004a and 2004b). Them both use $\boldsymbol{O}$ as the key control variable. Besides, EDTOC provides robustness against model uncertainties. Other known alternatives, to cope with parameter uncertainties, are: to use adaptive algorithms to identify the parameters and adapt accordingly the control strategy (Bastin and Dochain, 1990; Van Impe and Bastin, 1995; Van Impe, 1998) or to use Adaptive Extremum-Seeking strategies (Marcos *et al.*, 2004; Titica *et al.*, 2003) but again they both require, for the WWT case at hand, unavailable state measurements. Hence they are not considered here.

Table 1 lists the control strategies proposed to face the five SBR problems described when operated in FTC mode. This paper presents the comparison between these control strategies, considering the practical issues involved. Section 2 states the mathematical model of the SBR, Section 3 explains the control strategies to be compared, Section 4 summarizes the experiments performed and some conclusions close the paper.

Table 1. Comparison of the main problems tackled by different SBR control strategies (treating toxicants)

(FTC) Fixed Timing Control	**(VTC)** Variable Timing Control	**(OBTOC)** Observer Based Time Optimal Control	**(EDTOC)** Event Driven Time Optimal Control
None (usual)	Starvation Instrument	Starvation Instrument Optimality Peaks	Starvation Instrument Optimality Peaks Uncertainty

2. SBR MODEL

Equations (1-4) approximate the SBR model for the Filling and Reaction phases. Settling and Draw phases are of no relevance to the problems at hand.

$$\frac{dX}{dt} = \mu X - \frac{Q}{V}X \tag{1}$$

$$\frac{dS}{dt} = -k_1 \mu X + \frac{Q}{V}(S_i - S) \tag{2}$$

$$\frac{dV}{dt} = Q \tag{3}$$

$$\frac{dO}{dt} = -(k_2 \mu + b)X + K_l a(O_s - O) - \frac{Q}{V}O \tag{4}$$

$$\mu(S) = \frac{\mu_0 S}{K_S + S + S^2 / K_I} \tag{5}$$

States *X (g/L)*, *S (g/L)*, *V (L)* and *O (g/L)* represent Biomass, Substrate, Volume level and Dissolved Oxygen concentrations respectively, S_i *(g/L)* denotes the substrate concentration in the influent, k_1 and k_2 are yield coefficients, *b* is the endogenous respiration coefficient, *Q (L)* is the influent flow, the manipulated variable, μ *(h^{-1})* is the specific biomass growth rate, μ_o *(h^{-1})* is a parameter related to μ*, K_S is known as the saturation constant and K_I as the inhibition constant.

3. CONTROL STRATEGIES

Fig. 2(a2) shows the SBR TP-SV when FTC is used. Note that the horizontal part of the TP-SV indicates there is no filling ($\boldsymbol{V}$ keeps constant). In this condition the toxic substrate concentration $\boldsymbol{S}$ diminish because of biomass action. To assure that $\boldsymbol{S}$ gets below some final acceptable $\boldsymbol{S_f}$ before finishing the batch, some fixed time is allowed.

3.1. VTC (*Variable Timing Control)*

The variable timing control is similar to the FTC. Its TP-SV is exactly the same. The difference is that the reaction time is no longer fixed.

Fig. 2(a1) shows a Near-End Detection (NED) module that signals the end of the reaction using the $\boldsymbol{O}$ dynamics expressed in Eq. (4), without the need to measure $\boldsymbol{S}$. Note that after filling the SBR, for a given constant aeration rate, $\boldsymbol{O}$ will exhibit a unique minimum in time, closely related to the moment of maximum metabolic activity. Such maximum activity implies the maximum degradation rate and hence maximum $\boldsymbol{O}$ consumption. It happens just when $\boldsymbol{S}=\boldsymbol{S}^*$. When $\boldsymbol{O}$ rises again it is because activity decreases and $\boldsymbol{O}$ consumption diminishes, indicating the depletion of toxicant substrate. At this time the NED detects the end of the reaction and signals the sequencing module in Fig. 2(a1)) to proceed with the next phases to finish the batch.

3.2. OBTOC (*Observer based time optimal control)*

Observer based time optimal control is presented in Fig. 2(b1). Its ideal TP-SV is shown in Fig. 2(b2). Note it is exactly the same as TOC's. If $\boldsymbol{S}$ could be measured and if all parameters were perfectly known, including $\boldsymbol{S}_i$, it would be easy to implement the TOC. But that is not the case. Instead, OBTOC uses a *software sensor* to estimate $\hat{S}\approx\boldsymbol{S}$ by measuring $\boldsymbol{O}$ and $\boldsymbol{V}$.

Note that if OBTOC follows the ideal TP-SV it solves, simultaneously, some of the problems stated in the introduction. It delivers time-optimality without measuring $\boldsymbol{S}$. It also prevents inhibition to occur when toxic peaks arise in the influent (at least for known $\boldsymbol{S}_i$). As finishing time is known, starvation may also be prevented. However there are various drawbacks. The influent's substrate concentration ($\boldsymbol{S}_i$, not easily measurable either) needs to be known exactly. Also critical parameters need to be well known, as $\boldsymbol{S}^*$ for example. Even little mistakes in estimating these values affect the *software sensor* performance, causing the actual TP-SV to diverge from the TOC one. For this reason the OBTOC solution is considered non robust and hence difficult to successfully apply in practice.

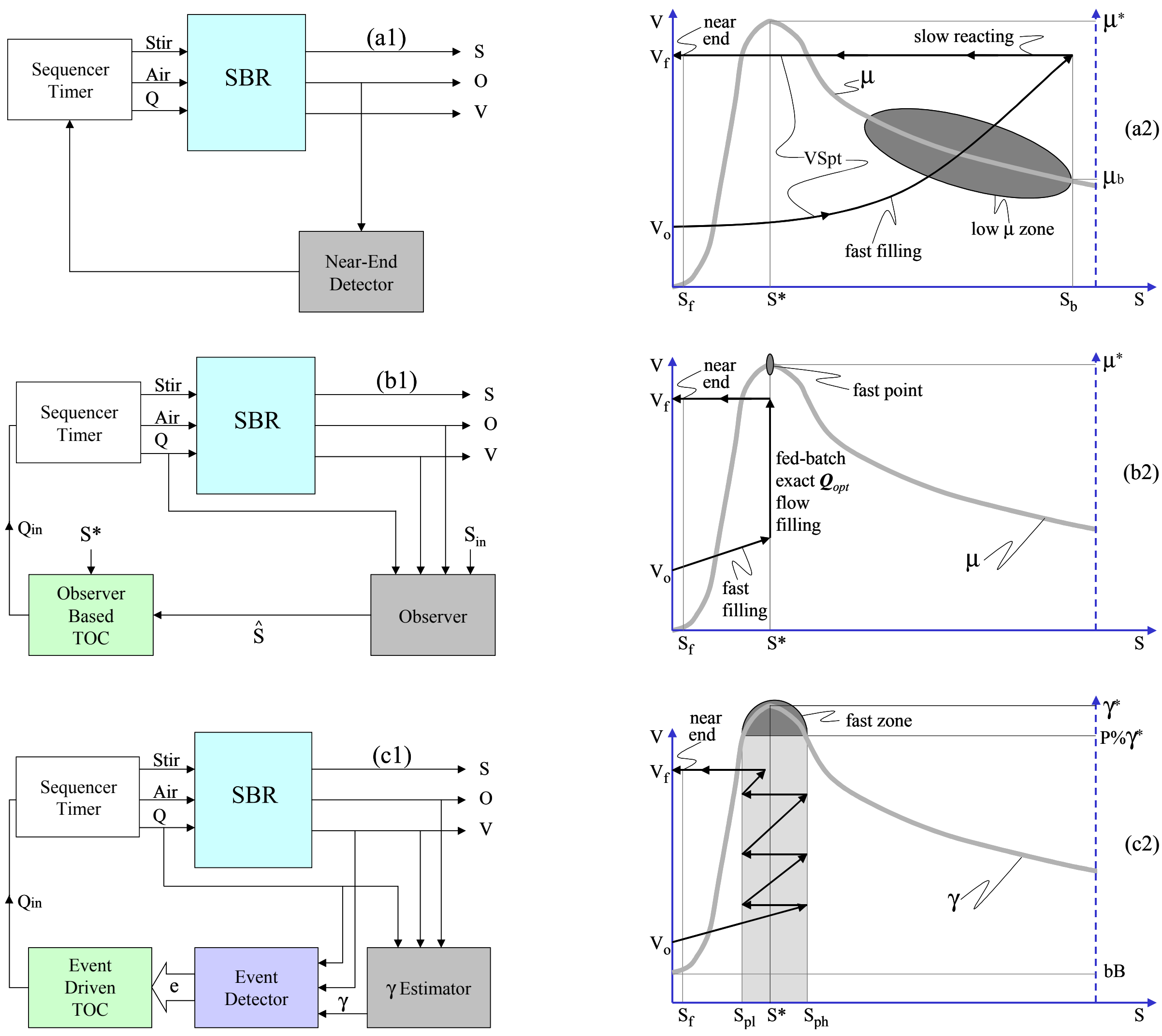

Figure 2. a) VTC, b) OBTOC, c) EDTOC; 1) Control Diagram, 2) Trajectory projection in S-V plane (TP-SV) Secondary axis is for $\boldsymbol{\mu}$ or $\boldsymbol{\gamma}$ respectively. Initial conditions $\boldsymbol{S}$=0 y $\boldsymbol{V}=\boldsymbol{V}_o$ are assumed. The dark area indicates the zone in which the process spends most of its reaction time.

3.3. EDTOC (Event driven time optimal control)

This method uses a different approach to cope with the lack of measurements and the uncertainties in model parameters while allowing operating the SBR in a near optimal way. The strategy is based on the following observations. In the OBTOC case, for the non singular arcs, bang-bang control implementation was robust against uncertainties and information requirement was low. The problem was implementing the singular arc solution. Our proposal is then to replace the smooth and sensible singular signal with a *bang-bang* one that maintains its trajectory near and around the singular ideal trajectory. The generated error may be made, theoretically, as little as desired (Moreno, 1999). Robustness is linked to the well known properties of sliding mode control (Khalil, 2002; Slotine and Li, 1991). The low information requirement is related to the fact that only the singular surface needs to be estimated in the state space. Such surface is associated to certain events that depend on internal variables. If such events could be *software-sensed* using the measurable variables, then a practical solution becomes feasible. Even more, if the singular surface is robustly related to such events, the solution will be robust against model uncertainties.

The EDTOC in Fig. 2(c1) does not measure $\boldsymbol{S}$, but estimates a variable (denoted γ) related to the substrate degradation rate. Such γ could be estimated in real-time using $\boldsymbol{O}$ and $\boldsymbol{V}$ with Formula (6), which is easily obtained multiplying Eq. (4) by $\boldsymbol{V}$ and naming the total biomass as $\boldsymbol{B}=\boldsymbol{XV}$.

$$\gamma = (k_2\mu + b)B = K_l a V(O_s - O) - QO + V\frac{dO}{dt} \qquad (6)$$

Compare μ and γ in Fig. 2(b2) and Fig. 2(c2). They do have the same shape and both have a global maximum for $\boldsymbol{S}=\boldsymbol{S^*}$. But the advantage of having γ is that its maximum can be detected in real time, without knowing neither $\boldsymbol{S}$ nor $\boldsymbol{S^*}$. That is why it is possible to manipulate the inflow $\boldsymbol{Q}$ in such a way that γ stays inside the “fast zone” of Fig. 2(c2). A similar zone exists for μ (not shown). Such zone resides above ***P%*** of the maximum. The hatched rectangle in Fig. 2(c2) allows to explain how to maintain $\boldsymbol{S}$ oscillating between some $\boldsymbol{S_{pl}}$ (*lower than* $\boldsymbol{S}$*) and some $\boldsymbol{S_{ph}}$ (*higher*) all the way during the SBR filling. Each time $\boldsymbol{S}$ is about to leave such range, an event is generated and then the EDTOC commutes $\boldsymbol{Q}$ (*on/off*) to prevent it. This explains the zigzag in the TP-SV. As $\boldsymbol{P}\rightarrow 100\%$ the zigzag will be finer and then the control behavior will be closer to the TOC. This solution works regardless of the $\boldsymbol{S_i}$ value and regardless uncertainties and/or changes in most of the SBR parameters.

Only parameters $\boldsymbol{K_l a}$ and $\boldsymbol{O_s}$ are required to estimate γ, and it is not necessary to known them exactly. That makes the EDTOC robust. Even more, an error increment in parameter values will degrade EDTOC performance only gradually, that is, if parameter values are given far from real values, EDTOC will still behave acceptably. This reason makes such solution a good candidate for practical use in industrial environments.

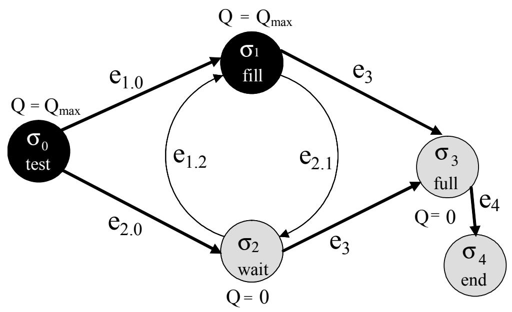

Figure 3. EDTOC finite state machine

Formally the EDTOC is represented by a finite state machine in Fig. 3, and the events that generate the state transitions are given in Table 2.

Tabla 2. EDTOC events for *fed-batch* processes

Event	Trigger	Estimates	Meaning
$e_{1.0}$	$d\gamma/dt>0$	$S<S^*$	NonInhibited
$e_{2.0}$	$d\gamma/dt<0$	$S>S^*$	Inhibited
$e_{2.1}$	$\gamma\leq P\gamma_K^*$	$S=S_{ph}$	Wait
$e_{1.2}$	$\gamma\leq P\gamma_K^*$	$S=S_{hl}$	Fill
$e_{3.}$	$V\geq V_{max}$	(measured)	TankFull
$e_{4.}$	$\gamma<\gamma_{end}$	$S<S_f$	ReactionEnd

Table 2 shows the events estimated by the event-detector in Fig. 2(c1). Using such events the EDTOC commutes the influent pump Q. Initial state for $k=0$ at $t = t_0 = 0$ is always σ_0. If inhibited, the system will instantaneously jump to state σ_2. After the initial *bang-bang* arc, cycling between σ_1 and σ_2 will approximate the singular arc of the optimal solution. Once the tank gets full, σ_3 will complete the last *bang-bang* arc. Reaction will be ended when σ_4 is reached and, after that, the remaining of the batch phases will take place.

4. EXPERIMENTAL RESULTS

A laboratory 7L pilot SBR was used. Sludge from a municipal WWTP was acclimated to treat synthetic wastewater containing 4-chloro-phenol (4CP). The standard toxicant concentration for these experiments was chosen to be $\boldsymbol{S_i}$=350mg4CP/L. Applying twice such concentration directly to the tank would inhibit and stress the biomass. Bigger concentrations in the tank may permanently disable the SBR.
A series of experiments was performed to determine the effect of the various control strategies on different problems, especially peak toxicant concentrations tolerance and time optimality. Previous to each experiment the SBR was acclimated and operated in FTC mode using the standard toxicant concentration.

In all VTC, OBTOC and EDTOC experiments the end of the reaction phase was successfully detected, thus no accidental starvation was ever registered.

For the OBTOC different observer configuration were tested in previous experiments. The best results were obtained using an extended Kalman filter, so this is the one used for this experiment series.

Results are presented in Figures 4 and 5. Figure 4 shows the toxicant removal efficiency R=($\boldsymbol{S}_i$-$\boldsymbol{S}_f$)/$\boldsymbol{S}_i$ when increasing toxicant input concentrations are applied. It can be seen that FTC and VTC strategies fail to remove all toxicant when its input concentration rises over 700mg/L and the SBR gets practically disabled for concentrations over 1400mg/L. OBTOC performs much better and keeps treating all the substrate up to concentrations of 1400mg/L. For higher $\boldsymbol{S}_i$ the OBTOC failed to keep the substrate concentration inside the SBR's tank in the expected range, so the experiments were stopped. That means that over such concentration uncertainties render the OBTOC useless, even when special care was put to estimate the SBR parameters as exactly as possible. EDTOC performance was even better. Total removal was achieved for all experiments performed up to the maximum allowable range of 11200 mg4CP/L (it was not possible to dilute higher concentrations for the given nutrients and toxicants). In short, the falling lines in Fig. 4 indicate the toxicant input concentration that renders each control strategy to a condition in which the SBR gets inhibited and no longer performs appropriately the toxicant removal treatment.

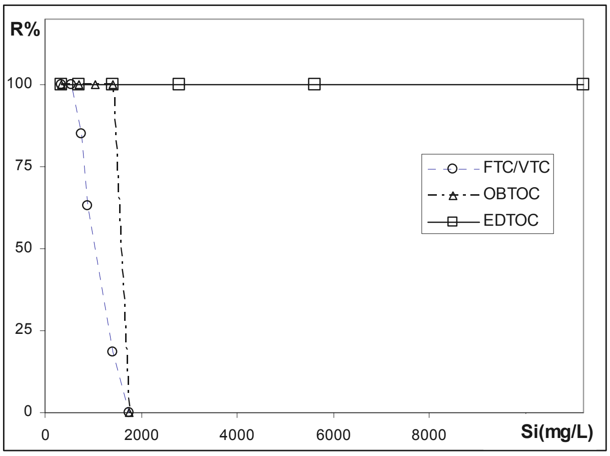

Figure 4. SBR toxicant removal efficiency (R%), for various input toxicant concentrations, using various control strategies. No data yet available for EDTOC for $\boldsymbol{S}_i$ higher than 11200 mg/L

Figure 5 gives an idea of the performance of the SBR operation. A comparison is made, for each control strategy, between the removal speed for the standard case and the removal speed when input toxicant peaks of increasing value are applied. It suggests that, in practice, for the experiments performed, EDTOC performs the best. In fact, independent measurements (not shown) confirm that at all times EDTOC maintained the substrate concentration $\boldsymbol{S}$ inside the SBR's tank at levels near the desirable $\boldsymbol{S}^*$, even for large $\boldsymbol{S}_i$ input peaks.

Experiments show that EDTOC was capable to cope with input peaks one order of magnitude higher than the ones tolerated by OBTOC, which in turn behaved in a superior way compared to FTC and VTC modes.

As the EDTOC is also a simple and robust strategy, it seems reasonable to dedicate some additional lines and graphs to analyze in detail one of its experiments.

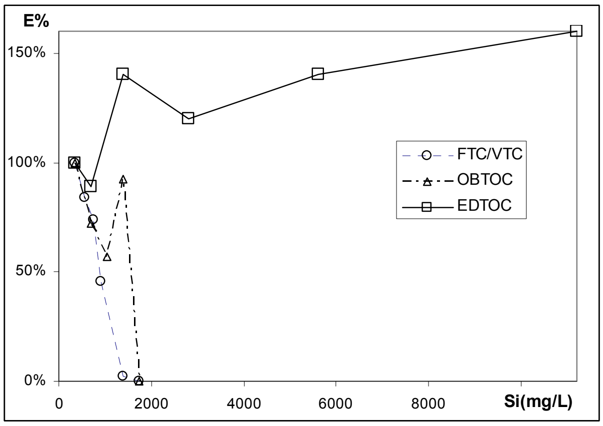

Figure 5. SBR relative efficiency (E%), for various input toxicant concentrations, using various control strategies. The average degradation rate is compared to the standard condition ($\boldsymbol{S}_i$ =350mg/L).

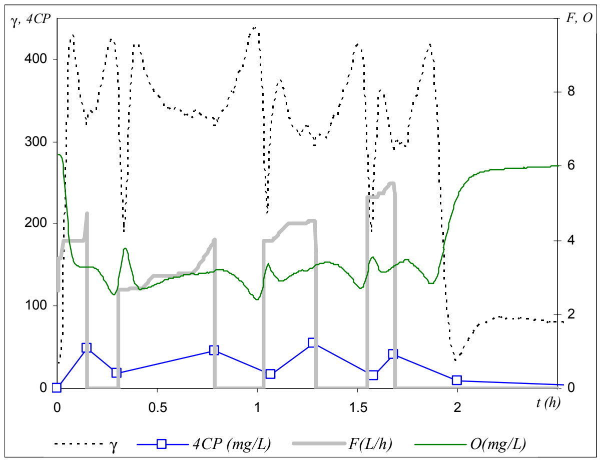

Figure 6. EDTOC experimental kinetics, case 14/07/2003; P = 0.9; Toxicant input concentration S_i = 634mg4CP/L

Fig. 6 shows the results for an experiment to treat 4CP. EDTOC was used, implementing γ from Eq. (5). Toxic substrate concentration inside the reactor $\boldsymbol{S}$ (see *4CP* in Fig. 6, square marks) was measured off-line, using manually taken samples. These values were not used with control purposes. Values up to $\boldsymbol{S}$=200mg/L are considered normal and safe for the biomass. An identification exercise later revealed $\boldsymbol{S}^*$ = 13.99 mg4CP/L ±7.4% for a confidence interval of 95%. Fig. 6 shows that $\boldsymbol{S}$ was kept oscillating around $\boldsymbol{S}^*$, in an acceptable concentration range. This was made by properly commuting *on* and *off* the influent's pump (Fig. 6, continuous thick line). Such behavior corroborates the effectiveness of the EDTOC strategy.

P=0.9 was chosen for all EDTOC experiments. Theoretically this implies a treatment time near to 5% higher than the optimal one.

Total biomass was $\boldsymbol{B}$=1.4g, exhibiting an increase of less than 2% for the whole reaction. Neither $\boldsymbol{B}$, $\boldsymbol{S}$, $\boldsymbol{S}_i$ nor $\boldsymbol{S}^*$ values were used by the controller.

It must be noted that an additional perturbation is provided by the sensor used to measure the Dissolved Oxygen concentration (Fig. 6, thin continuous line). The sensor introduces some noise, and second order delays, to state variable $\boldsymbol{O}$. This means that distortion and delays are to be expected when calculating γ from Eq. (5) (Fig. 6, dotted line) to use it in EDTOC. But, thanks to EDTOC robustness, the system did cope with all these perturbations and uncertainties.

5. CONCLUSIONS

From comparing different control strategies for toxic wastewater treatment (WWT) in sequencing batch reactors (SBR), and from experimental results, so far it is possible to draw some important conclusions:

Starvation at the end of a SBR batch cycle, an undesirable time period in which biomass lacks feeding that may happen when using the fixed timing control (FTC), could be avoided by applying either variable timing control (VTC), observer based time optimal control (OBTOC) or event based time optimal control (EDTOC).

Actual instrumentation limitations could be avoided if, instead of trying to measure Toxicant Substrate concentrations, Dissolved Oxygen concentration is measured, and then *software-sensor* are used to obtain the necessary information for control.

Uncertainties in the model and parameters affect the OBTOC, but are no problem for the EDTOC. The tradeoff is that EDTOC will always be sub-optimal even if the SBR model is perfectly known. In practice, however, EDTOC behaved better than OBTOC.

Input toxic concentration peaks are a problem for the FTC and VTC strategies. OBTOC can cope with peaks up to 1400mg4CP/L, while EDTOC behaves well for concentration one order of magnitude higher.

Strategies as the OBTOC and specially the EDTOC increase the performance of the SBR to levels never attained before. Research to further develop such operation modes is very promising. However, more experiments should be performed to finish this study. Long term biological stability should be addressed for the SBR when operated in Time Optimal Control (TOC) modes before categorically stating its benefits. This includes specially a study of the biological properties of the biomass when continuously subjected to this type of strategies.

ACKNOWLEDGEMENTS

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The scientific responsibility rests with the authors.

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Control y Mejoras en Biorreactores para Tratar Aguas Residuales Tóxicas

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Resumen

Se presentan alternativas para solucionar problemas asociados a la operación de biorreactores buscando que su desempeño sea cercano al óptimo, en especial el problema de tratar picos altos y desconocidos de concentración de tóxicos. Dos filosofías de solución se han ensayado experimentalmente. Una modifica la configuración de biomasa en el reactor. La otra consiste en mejorar las acciones de control. Se considera que el modelo del biorreactor puede conocerse de manera apenas aproximada y que, debido a las características técnico-económicas de la aplicación, no es posible medir muchas de las variables de interés, por lo cual existe poca información para el control del proceso.

1. INTRODUCCIÓN

El tratamiento biológico de aguas residuales con alta concentración de compuestos tóxicos, tal como las producidas por las industrias químicas y petroquímicas, es una tarea difícil, importante y retadora. Los biorreactores secuenciales por lotes (SBR por sus siglas en inglés, *sequencing batch reactor*) han demostrado su superioridad con respecto a los reactores continuos gracias a su mayor eficiencia y flexibilidad. El término SBR se usa ahora como sinónimo de la tecnología en Plantas de Tratamiento de Aguas Residuales (PTAR) donde el volumen del reactor es variable [13]. Pueden trabajar con biomasa suspendida o fija (a un soporte). En general los procesos SBR presentan 3 características: Repetición periódica de una secuencia definida de fases, duración definida de cada fase de acuerdo a los resultados que se pretendan lograr, y desarrollo dinámico de las reacciones biológicas y físicas como funciones del tiempo. Sin embargo su operación básica enfrenta algunos problemas clave:

1. La relación entre la concentración del tóxico y la eficiencia de la planta es no lineal y de carácter inhibitorio. Esto ocasiona un mal desempeño de la PTAR si se somete a incrementos súbitos (picos) de la concentración tóxica a tratar. Dichos picos son frecuentes debido por ejemplo a una operación industrial intermitente.

2. La naturaleza tóxica del sustrato hace necesaria una aclimatación previa de la biomasa. Del mismo modo, un ayuno prolongado de biomasa ya aclimatada altera sus cualidades biológicas. Estos ayunos pueden presentarse al aplicar las políticas comunes de operación de PTARs [3, 5].

3. El control óptimo de un SBR requiere la medición en línea de la concentración tóxica. Sin embargo esto no es implementable en la práctica, hoy día, por razones técnico-económicas.

El objetivo de este artículo es presentar varias ideas implementadas por nuestro grupo para intentar solucionar estos problemas. Experimentalmente se han ensayado dos vías, tal como lo representa la Tabla 1. De un lado la mejora de estrategias de control basadas en la medida de Oxígeno Disuelto (OD), las cuales se discutirán en la Sección 2. De otro lado la alteración de la configuración de la biomasa dentro del reactor, explicadas en la Sección 3. La Sección 4 resume los experimentos realizados. Las conclusiones cierran el artículo.

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Tabla 1. Vías de Investigación Experimental. Se referencian los problemas analizados y se sugieren Futuros Experimentos (FE)

Modo de Control / Config de la Biomasa	FTC Fixed Timing Control	VTC Variable Timing Control	OBTOC Observer Based Time Optimal Control	EDTOC Event Driven Time Optimal Control
BS: Biomasa Suspendid	Picos - Ayuno- Inhibi	Picos - Inhib Usa OD	Picos+ Inhib Usa OD	Picos++ Inhib Usa OD
BM: Biomasa Móvil	Picos Ayuno+ Inhib	FE	FE	FE
BF: Biomasa Fija	Picos Ayun++ Inhib	FE		

2. ESTRATEGIAS DE CONTROL

Muchos procesos de fermentación industriales utilizan biorreactores. La forma de control más simple y difundida en SBRs es el lazo abierto (FTC en la Tabla 1), con tiempos fijos para cada fase (llenado, reacción, sedimentación, vaciado y ayuno ó tiempo muerto). Dado que es razonable optimizar el funcionamiento de dichos procesos, se han diseñado métodos de control realimentado, apoyados en el modelo aproximado dado por las Ecuaciones (1-4), para disminuir el tiempo dedicado a las fases de llenado-reacción. El más sencillo consiste en detectar el fin de la reacción (VTC en Tabla 1) aprovechando la dinámica del OD.

También se ha usado la teoría de control óptimo para determinar la mejor política de control [8, 9, 11]. Pero dado que la medida de la concentración de sustrato resulta impráctica, el OD se mide en su lugar, dando origen a dos estrategias de control próximas al óptimo teórico, la de tiempo óptimo basada en observadores (OBTOC en Tabla 1) y la basada en eventos (EDTOC en Tabla 1).

2.1. FTC (*Fixed Timing Control)*

El control de tiempos fijos es la estrategia usual en la cual un experto fija los tiempos de cada fase según su experiencia y según los valores esperados de las concentraciones.

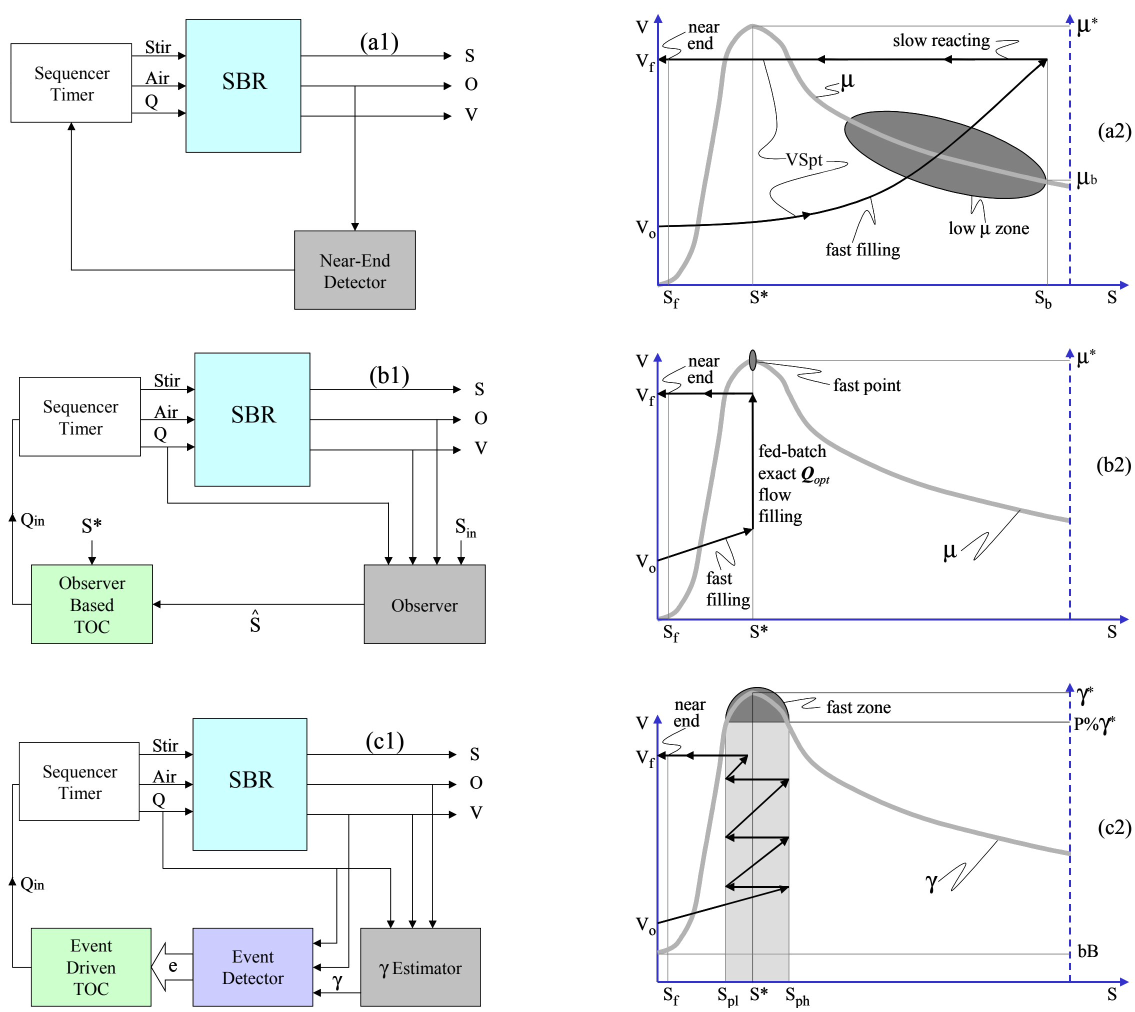

Figura 1. a) VTC, b) OBTOC, c) EDTOC; 1) Diagrama de Control, 2) Proyección de la Trayectoria del sistema en el plano S-V ; Eje secundario para μ ó γ respectivamente. El área oscura marca la zona en la cual el proceso invierte la mayor parte del tiempo de reacción. Se asumen condiciones iniciales S=0 y V=V_o

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Si el tiempo asignado para reacción es poco, el reactor no terminará de degradar el sustrato y, el agua aún tóxica será vertida al finalizar el lote. Si el tiempo es mayor al necesario, el proceso perderá eficiencia. Sin embargo, por seguridad, normalmente el tiempo asignado es mucho mayor al necesario.

La evolución de la proyección de la trayectoria del sistema en el eje Sustrato-Volumen (SV) se aprecia en la Figura 1(a2). En este caso el llenado se realiza usando el máximo flujo posible, lo cual explica por qué este método carece de robustez ante picos de concentración, dado que la máxima concentración del tóxico dentro del reactor, S_b, dependerá directamente de la concentración del influente (agua tóxica en la entrada). Este mismo hecho hace que la inhibición sea la situación normal de operación, dado que típicamente S_b es mayor que la concentración óptima $\boldsymbol{S}^*$. Nótese que la parte horizontal de la trayectoria SV indica que no hay llenado del tanque ($\boldsymbol{V}$ constante). En esa condición el sustrato tóxico disminuye debido a la metabolización por parte de la biomasa. Sin embargo, la mayor parte del tiempo dicha concentración permanece por encima del punto óptimo, es decir, inhibiendo la biomasa.

2.2. VTC (*Variable Timing Control)*

El control de tiempo variable [4] es similar al FTC y su proyección SV es exactamente igual (Fig. 1(a2)). La diferencia es que el tiempo asignado a la reacción no es fijo, sino que varía en función de la determinación del final de reacción. El esquema se aprecia en la Fig. 1(a1). Allí se destaca el módulo detector de cuasi-final de reacción (NED). Este se basa en la dinámica del OD según el modelo matemático del reactor expresado en las Ecuaciones (1-4), particularmente en la Ecuación (4). Allí los estados X *(g/L)*, S *(g/L)* y O *(g/L)* representan las concentraciones de biomasa, sustrato y oxígeno disuelto (OD) respectivamente, μ (h^{-1}) es la tasa especifica de crecimiento de biomasa, S_i *(g/L)* denota la concentración de sustrato en el influente, k_1 y k_2 son coeficientes de producción, b el coeficiente de respiración endógena, Q *(L)*, la variable de control manipulada, es el flujo y V *(L)* es el volumen del medio liquido en el tanque.

$$\frac{dX}{dt} = \mu X - \frac{Q}{V} X \tag{1}$$

$$\frac{dS}{dt} = -k_1 \mu X + \frac{Q}{V}(S_i - S) \tag{2}$$

$$\frac{dV}{dt} = Q \tag{3}$$

$$\frac{dO}{dt} = -(k_2 \mu + b)X + K_l a(O_s - O) - \frac{Q}{V} O \tag{4}$$

Luego del llenado, y dada una aeración constante del tanque del reactor, el OD tendrá un único mínimo temporal, el cual se asocia al momento cuando la concentración de sustrato posibilita la máxima actividad metabólica de la biomasa y por tanto la máxima degradación de sustrato. Dicho mayor consumo de OD sucede para valores relativamente bajos de sustrato ($\boldsymbol{S}^*$). Por tanto si, posterior al mínimo, el valor de oxígeno vuelve a subir a valores cercanos a saturación, esto indica que ha disminuido la actividad metabólica por ausencia de sustrato (tóxico), $\boldsymbol{S} \leq \boldsymbol{S}_f$, y la reacción ya está prácticamente terminada. Es allí que el NED detecta que la reacción ha terminado y envía la señal al módulo de secuencia y temporizado (Fig. 1(a1)) para que, luego de un tiempo adicional de seguridad, prosiga con las demás fases del lote.

2.3. OBTOC (*Observer based time optimal control)*

El control de tiempo óptimo basado en observadores [12] se presenta en la Fig. 1(b1) y la proyección SV de la trayectoria óptima en la Fig. 1(b2) [8]. Esta trayectoria consiste de tres arcos cuando se consideran los límites naturales del actuador (bomba del influente). En el primer arco *bang-bang* se llena el reactor rápidamente (flujo máximo) hasta lograr la concentración optima $\boldsymbol{S}^*$. Luego en el segundo arco, el singular, se aplica un flujo de entrada $\boldsymbol{Q}_{in}=\boldsymbol{Q}_{opt}$, justo el necesario para mantener $\boldsymbol{S}=\boldsymbol{S}^*$ hasta llenar el reactor. De allí el tramo vertical de la trayectoria, lo cual significa que no se presentan cambios en $\boldsymbol{S}$ a medida que se incrementa $\boldsymbol{V}$. Y el último arco *bang-bang* consiste simplemente en esperar, sin agregar influente, hasta que la reacción termine. Si fuese posible medir $\boldsymbol{S}$, y se conocieran sin incertidumbre todos los parámetros del sistema, el arco singular se realizaría fácilmente con un controlador estándar. Sin embargo, como no es ese el caso, el uso de un observador (*software sensor*) que utilice el OD para estimar $\hat{S} \approx \boldsymbol{S}$ permite solucionar teóricamente el problema. El inconveniente es que se necesita conocer exactamente la concentración del sustrato en el influente ($\boldsymbol{S}_i$, que tampoco es fácilmente medible) y también es necesario conocer los parámetros críticos del SBR, tal como $\boldsymbol{S}^*$ por ejemplo. Un pequeño error en la estimación de estos valores ocasiona un pobre desempeño del observador y por tanto la proyección SV de la trayectoria real no reflejará a la óptima. Es por esta razón que la solución OBTOC es poco robusta y difícil de aplicar en la práctica.

2.4. EDTOC (*Event driven time optimal control)*

En este método se usa una actitud diferente para combatir la falta de mediciones y la incertidumbre del modelo, al mismo tiempo que se propende por optimizar la operación del biorreactor La idea principal se basa en la siguiente observación. Tal como se explicó en el numeral anterior para el OBTOC, cuando la solución no singular puede implementarse con realimentación los requerimientos de información son bajos y su implementación es robusta ante incertidumbres del modelo. El problema reside en la determinación e implementación del arco singular el cual requiere un buen conocimiento del modelo y parámetros de la planta y es sensible a incertidumbres. En este método se propone reemplazar la suave y sensible señal de control singular por una *bang-bang* que

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mantenga la trayectoria alrededor de la superficie singular. El error generado puede hacerse tan pequeño como se desee (teóricamente) [6, 8]. La robustez de esta implementación está ligada a las bien conocidas propiedades de modos deslizantes [7, 10]. El bajo requerimiento de información se relaciona con el hecho de que solamente es necesario determinar la superficie singular en el espacio de estado. Dicha superficie está asociada a ciertos eventos de las variables internas. Si tales eventos pueden ser sensados (*software-sensed*) usando exclusivamente las variables medibles, entonces una solución práctica es posible. Si adicionalmente la superficie singular se relaciona robustamente con los eventos, la solución será robusta ante incertidumbres del modelo. Es así que el control de tiempo óptimo basado en eventos [1, 2] de la Fig. 1(c1) soluciona el problema de robustez, no midiendo $\boldsymbol{S}$, sino calculando una variable (denominada γ) relacionada con la velocidad de reacción. Tal γ puede estimarse en tiempo real utilizando el OD (O) y el Volumen (V) con la Fórmula (5).

$$\gamma = (k_2\mu + b)B = K_l a V(O_s - O) - FO + V\frac{dO}{dt} \qquad (5)$$

Compare γ y μ en la Fig. 1(c2) y Fig. 1(b2). Tienen la misma forma. Es por ello que resulta posible manipular $\boldsymbol{Q}_{in}$ de forma que la velocidad de reacción permanezca dentro de una "zona rápida" en la Fig. 1(c2). Tal zona se encuentra por encima de un ***P%*** de la máxima velocidad. Asociada a dicha zona existe un rectángulo sombreado con el cual se explica como controlar $\boldsymbol{S}$ de modo que oscile en un rango entre algún $\boldsymbol{S}_{pl}$ (*lower than* $\boldsymbol{S}$*) y $\boldsymbol{S}_{ph}$ (*higher*) durante todo el llenado del SBR. Cada vez que $\boldsymbol{S}$ intenta salir de este rango, un evento es generado y entonces el EDTOC conmuta $\boldsymbol{Q}_{in}$ (*on/off*), para prevenirlo. Es por esto que la proyección SV de la trayectoria zigzaguea dentro del sombreado. A medida que $\boldsymbol{P}\rightarrow 100\%$ el zigzag será mas fino y entonces el comportamiento del control se aproximará al óptimo teórico. Esta solución funciona sin importar el valor de $\boldsymbol{S}_i$ y a pesar de los cambios en la mayoría de los parámetros del SBR

Únicamente son necesarios $\boldsymbol{K}_l a$ y $\boldsymbol{O}_s$ para estimar γ, y aún estos no necesitan conocerse exactamente. Es por ello que el EDTOC es robusto. Adicionalmente, un incremento del error de estimación en dichos parámetros degradará el desempeño del EDTOC sólo de manera gradual. Aún si los parámetros se obtienen alejados de su valor real, el EDTOC se comportara de manera aceptable. Por tal razón esta solución es una buena candidata para usos en ambientes industriales.

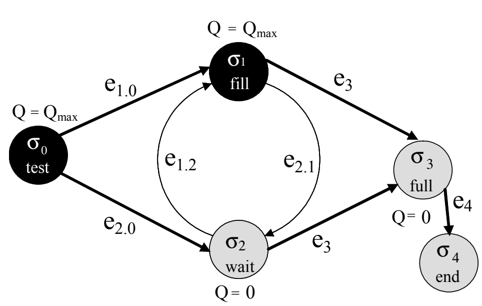

Figura 2. Máquina de estados finitos del EDTOC

Formalmente el EDTOC puede representarse por la máquina de estados finitos de la Fig. 2, y los eventos que generan las transiciones entre estados se resumen en la Tabla 2.

Tabla 2. Eventos para procesos *fed-batch* en un SBR

Evento	Trigger	Estimación	Significado
$e_{1.0}$	$d\gamma/dt>0$	$S < S^*$	No Inhibido
$e_{2.0}$	$d\gamma/dt<0$	$S > S^*$	Inhibido
$e_{2.1}$	$\gamma \leq P\gamma_K^*$	$S = S_h$	Esperar
$e_{1.2}$	$\gamma \leq P\gamma_K^*$	$S = S_l$	Llenar
$e_{3.}$	$V \geq V_{max}$	(medido)	TanqueFull
$e_{4.}$	$\gamma < \gamma_{end}$	$S < S_{end}$	FinReacción

La Tabla 2 muestra los eventos estimados por el detector de eventos de la Fig. 1(c1). Usando dichos eventos el EDTOC conmuta la bomba de influente Q. El estado inicial para $k = 0$ en $t = t_0 = 0$ es siempre σ_0. Si se inhibe, el sistema saltará instantáneamente al estado σ_2. Luego del arco *bang-bang* inicial, el ciclo que se forma entre σ_1 y σ_2 aproximará el arco singular de la solución óptima. Una vez el tanque se llena, σ_3 completará el último arco *bang-bang*. La reacción terminará al alcanzar σ_4 luego de lo cual se continuará con las demás fases del lote.

3. CONFIGURACIÓN DE BIOMASA

El reactor fue inoculado con microorganismos provenientes de una planta de tratamiento municipal de lodos activados (2000 mgVSS/L) manteniendo una retención celular de 20 días. Se usaron 3 alternativas de configuración de la biomasa: Biomasa suspendida (BS), Biomasa Móvil (BM), que se compone de una mezcla una mezcla de biomasa suspendida y biomasa fija por colonización de empaques de polietileno de alta densidad (con un área superficial de 963 m2/m3), y Biomasa Fija (BF) la cual utilizó como material de soporte una roca volcánica porosa (puzolana) con porosidad de 63% y diámetro medio entre 1.0 y 1.5 cm.

Como puede verse en la Tabla 1 los experimentos que incluyen mejoras al control del reactor se hicieron únicamente para la configuración BS (biomasa suspendida) logrando significativa mejoras en la tolerancia a picos de concentración. Sin embargo se mencionan las demás configuraciones debido al interés que plantean para futuros trabajos en control, especialmente porque presentan mejor resistencia al ayuno, es decir, a no perder su capacidad degradadora por el hecho de permanecer largos periodos de tiempo sin alimentación de sustrato.

4. EXPERIMENTOS

Se utilizó un biorreactor piloto de laboratorio de 7L aclimatado con lodos provenientes de una planta de tratamiento municipal para degradar agua sintética conteniendo 4-chloro-phenol (4CP) ó una mezcla de compuestos fenólicos en igual proporción (phenol, 4CP, 2,4-dichlorophenol, and 2,4,6-trichlorophenol). La concentración usual de tóxico para procesamiento en SBR es de S_i=350mg4CP/L. Aplicar mas del doble de dicha cantidad inhibiría fuertemente y estresaría a la biomasa, incrementando el tiempo de tratamiento de manera no lineal. Aplicar mayores concentraciones puede inhibir y/o deshabilitar al reactor permanentemente.

Se realizó una serie de experimentos para determinar el efecto de los diferentes tipos de control y diferentes configuraciones de biomasa en las características del sistema, especialmente resistencia al ayuno, a la inhibición, y a las concentraciones pico de sustrato. Lo resultados de esta última serie de experimentos se presentan en la Tabla 3. Para cada experimento el reactor se aclimató y operó previamente a la concentración estándar y utilizando la estrategia FTC. Una vez realizado el experimento respectivo, se regresa de inmediato al modo estándar de operación para medir el efecto inhibitorio de corto plazo, comparando la reacción anterior y la reacción posterior al experimento (última columna de la Tabla 3: (Qe/Qa). Allí se aprecia que el reactor sufre en su desempeño posterior al pico de concentración para las estrategias FTC y VTC, y que incluso para concentraciones de 1400mg/L la VTC sufre drásticamente en su operabilidad.

Para el OBTOC se estudiaron diferentes tipos de observador, obteniéndose mejores resultados con un filtro de Kalman extendido, el cual se utilizó. Puede verse en la última columna de la Tabla 3 (Qe/Qa) que el pico con OBTOC no tiene prácticamente efecto en la operación a corto plazo del SBR. Lo mismo puede decirse para la EDTOC. Analizando la antepenúltima columna que indica la eficiencia (optimalidad) de remoción del sustrato tóxico (Qu) se aprecia como la EDTOC alcanza los mayores niveles incluso para altísimos picos de concentración.

Los valores máximos de pico de concentración presentados para cada caso son los valores máximos a los cuales la estrategia se pudo poner en operación sin riesgo para el SBR. Esto muestra que la estrategia EDTOC pudo controlar adecuadamente picos de concentración un orden de magnitud por encima del máximo del OBTOC. Por tal razón, y en virtud de ser una estrategia más simple y robusta, se dedicará un espacio adicional a analizar con detalle una de las cinéticas experimentales EDTOC.

La Fig. 3 muestra una cinética experimental para degradar 4CP, usando γ en la Ecuación (5) para implementar el EDTOC. La concentración de sustrato tóxico $\boldsymbol{S}$ al interior del biorreactor (ver *4CP* en Fig. 3, marcas a cuadros) fue medida fuera de línea, usando muestras tomadas manualmente, y no fue usada con propósitos de control. Hasta un valor de S=200mg/L se considera normal y seguro para la biomasa. Un ejercicio de identificación posterior reveló un valor óptimo S^* = 13.99 mg4CP/L ±7.4% para un intervalo de confianza del 95%. La Figura 3 muestra que $\boldsymbol{S}$ fue mantenida en oscilación alrededor de $\boldsymbol{S^*}$, en un aceptablemente bajo rango de concentración, al conmutar adecuadamente *on/off* la bomba de influente (Fig. 3, línea continua gruesa). Este comportamiento muestra la efectividad de la estrategia EDTOC.

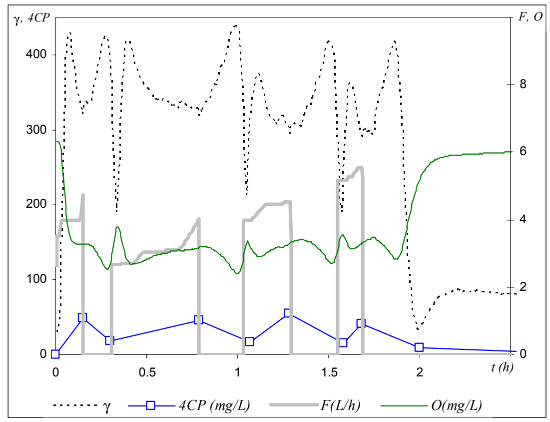

Figura 3. Cinética experimental EDTOC, caso 14/07/2003; P.=.0.9; Concentración de tóxico en el influente S_i.=.634mg4CP/L

La biomasa fue de B=1.4g exhibiendo un incremento de menos de un 2% durante la reacción. Su valor no fue usado por el controlador. Tampoco se usaron los valores de S, S_i ni S^*. Una perturbación adicional proviene del sensor usado para medir el Oxígeno Disuelto (Fig.3, Línea delgada continua). Este introduce efectos apreciables de Segundo orden, y algo de ruido, a la variable de estado O. Por tanto es de esperarse que se presenten distorsiones y retardos al calcular γ en la Ecuación (5) (Fig. 3, línea punteada) para usarla en el EDTOC. Pero gracias a la robustez del EDTOC el sistema toleró todas estas perturbaciones e incertidumbres.

Al realizar una serie de experimentos en la cual se aumentaba gradualmente la concentración de tóxico en el influente (hasta 11.2g4CP/L), usando la estrategia EDTOC para controlar el SBR, se observó un incremento lineal del tiempo de tratamiento con respecto a S_i. Se observó también que la biomasa jamás estuvo sometida ni a inhibición ni a estrés, pues en el interior del reactor la concentración fue siempre menor a 100mg4CP/L. Para los experimentos se escogió P = 0.9 lo cual, en teoría, implica un tiempo de tratamiento solamente un 5% mayor que el óptimo.

5. CONCLUSIONES

De los resultados obtenidos hasta ahora se obtienen, dos importantes conclusiones:

1. Si no se utilizan estrategias especiales de control entonces los sistemas que incluyen biomasa soportada, Móvil o Fija (BM ó BF), tienen

Tabla 3. Efecto de diferentes estrategias sobre el desempeño del reactor sometido a picos de concentración

Estrategia de Control	Tipo de Biomasa	Pico de 4CP, mg/L (S_{in})	Eficiencias durante el pico (%)	**Qa:** Tasa de degradación antes del pico (mg 4CP/gVSS-h)	**Qu:** Tasa de degradación durante el pico (mg 4CP/gVSS-h)	**Qe**:Tasa de degradación después del pico (mg 4CP/gVSS-h)	Efecto del pico: Relación de degradación (**Qe/Qa**)
FTC	BS	550	100	25.0	21.0	22.2	0.9
		760	85	25.0	18.5	11.3	0.5
		900	63	25.0	11.4	7.4	0.2
VTC	BS	700	100	59.8	44.9	59.8	1.0
		1050	100	59.8	9.0	18.0	0.3
		1400	18.3	59.8	0.9	N.D.	N.D.
OBTOC	BS	700	100	79.3	57.1	79.3	1.0
		1050	100	79.3	45.1	79.3	1.0
		1400	100	79.3	73.3	79.3	1.0
EDTOC	BS	700	100	71.4	63.5	71.4	1.0
		1400	100	65.0	91.2	71.4	1.1
		2800	100	95.3	114.3	101.5	1.1
		5600	100	81.6	114.3	71.4	0.9
		11200	100	71.4	114.3	64.5	1.0

N.D. No se pudo adquirir datos suficientes para computar (muy baja: el SBR quedó afectado por el experimento)

mayor resistencia al ayuno y a picos de concentración que la configuración de biomasa suspendida (BS). Sin embargo la diferencia no es suficientemente grande como para considerarlas una solución ante condiciones de operación extremas del SBR.

2. Estrategias de control como la OBTOC y la EDTOC incrementan sustancialmente la robustez y desempeño del SBR a niveles nunca obtenidos antes sin ellas. La investigación para desarrollar tales modos de control es por tanto muy prometedora.

Más experimentos deben realizarse para terminar este estudio. Debe estudiarse la estabilidad de largo plazo (biológica) del SBR sometido a estrategias TOC antes de poder afirmar categóricamente la bondad de sus propiedades. Esto incluye especialmente un estudio de la evolución de las propiedades de la biomasa bajo este tipo de estrategias. Nuestra hipótesis es que la combinación de biomasa suspendida y biomasa fija (Biomasa Móvil) combinada con la estrategia EDTOC dará los mejores resultados para el sistema completo.

AGRADECIMIENTOS

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Experiment 3 realized by WP1 to test control strategies provided by WP5

(Fragment taken from WP1 report, Partner 6, UNAM)

Evaluation of the process improvement with the application of the suboptimal EDTOC strategy by comparison with a non optimal (FTC) strategy. Application of shock loads.

The evaluation of the process improvement with the application of the ED-TOC strategy by comparison with a non optimal (FTC) strategy in the degradation of shock loads was realized comparing the time needed to degrade four quantities of 4CP (1.4, 12, 20, 28 g). For the ED-TOC strategy, the dilution of these quantities was in 4 L in order to be applied in a single batch. Thus taking into account this dilution the following influent concentrations were obtained: 350, 3000, 5000 and 7000 mg 4CP/L.

3.1.1. Degradation of 4CP by FTC strategy

The reactor operating under the FTC strategy degraded 1.4 g of 4CP (S_i in the influent of 350 mg/L) in 1 cycle of 4h. For the FTC strategy this is the best situation since for higher substrate concentrations, inhibition of the biomass occurs (Buitrón *et al*. 2003). Figure 13 shows a typical FTC degradation kinetic of de 1.4g of 4CP in the SBR.

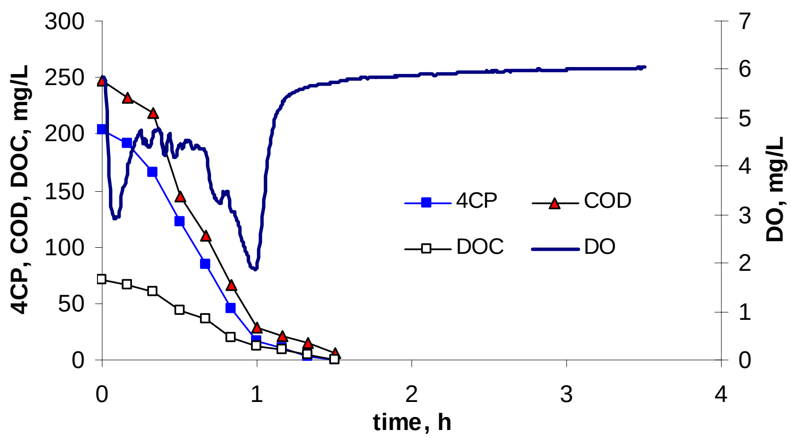


***Figure 13**. Behavior of the substrate concentration, measured as 4CP, COD, and DOC during the degradation of 1.4g 4CP using the FTC strategy*

The time required for the degradation of the different quantities of 4CP under the FTC strategy was evaluated considering that the optimal quantity that the volume of the reactor can degrade is 1.4 g, i.e., 1.4 g/7L or 350 mg/L. Thus several cycles of the SBR are required, due to the fact that a higher quantity of 4CP must be diluted in order to be efficiently degraded under the FTC strategy.

Thus, the time necessary to degrade the amounts of 4CF by the FTC strategy are the following ones:

1.4 g of 4CP = 4 hours (1 cycle)
12 g of 4CP = 36 hours (9 cycles)
20 g of 4CP = 60 hours (15 cycles)
28 g of 4CP = 80 hours (20 cycles)

3.1.2. Degradation of 1.4 g 4CP by the ED-TOC strategy

The degradation of 1.4g 4CP was made in 2h (the total cycle was 3.5h), Figure 14 presents the behavior of the substrate concentration, measured as 4CP, COD, and DOC during a cycle. It is possible to distinguish how the control operates if the substrate evolution and the DO curve are followed. The quantity of 4CP never was superior to 50mg/L, due to the ED-TOC strategy operating around S*

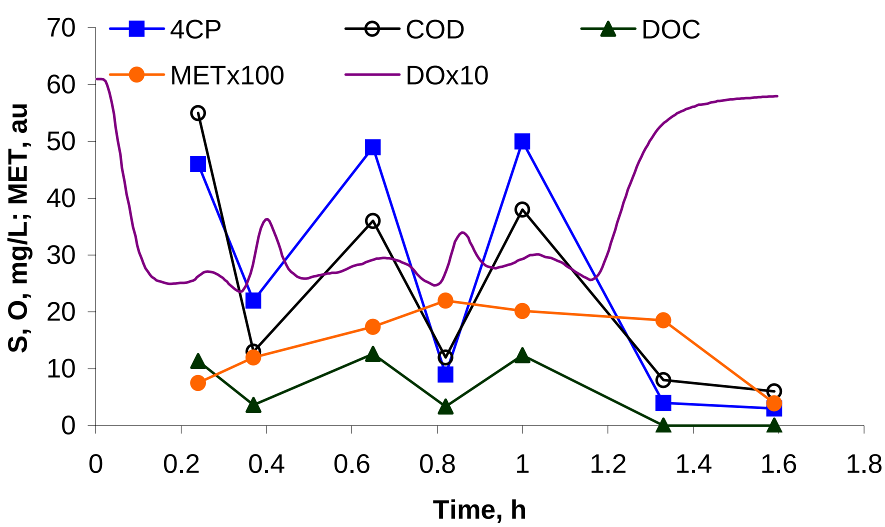


Figure 14. *Behavior of the substrate concentration, measured as 4CP, COD, and DOC during the degradation of 1.4g 4CP using the ED-TOC strategy*

3.1.3. Degradation of 12 g 4CP by the ED-TOC strategy

The degradation of 12g 4CP was made in 24h (the total cycle was 26h), Figure 15 presents the degradation during a cycle. It is possible to distinguish how the control operates if the substrate evolution and the DO curve are followed. In the figure it is possible to observe that, during the cycle, the filling is stopped when the DO increases indicating the maximal degradation rate in the Haldane curve has been passed. At this moment the fill is stopped and the 4CP is degraded. In the reactor, the quantity of 4CP never was superior to 50mg/L, except in the first filling period (the first mini-batch) 70mg/L where the ED-TOC strategy try to adapt the inflow to find S* (around 20mg/L).

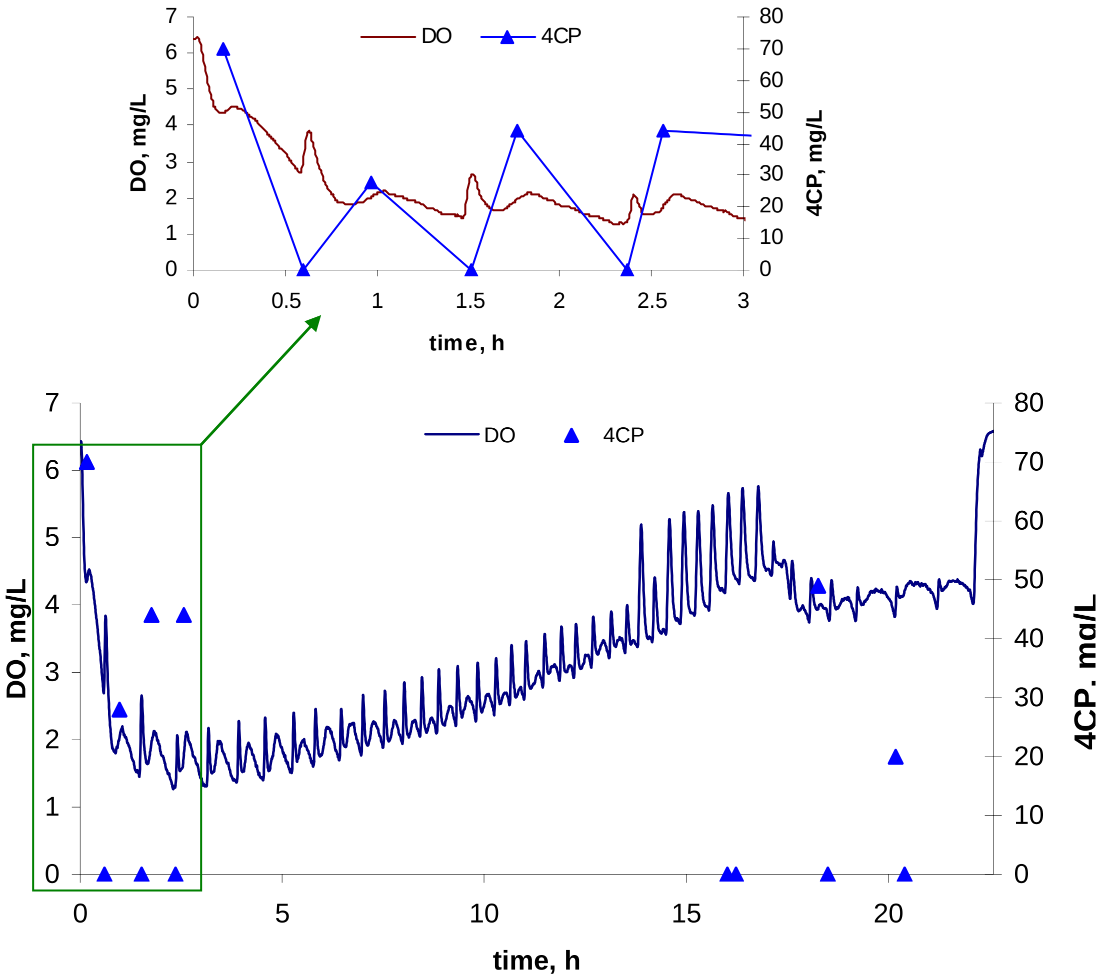


Figure 15. *Behavior of the substrate concentration, measured as 4CP, COD, and DOC during the degradation of 12g 4CP using the ED-TOC strategy*

3.1.4. Degradation of 20 g 4CP by the ED-TOC strategy

The degradation of 20g 4CP was made in 30h (the total cycle was 31h), Figure 16 presents the degradation during the cycle. The quantity of 4CP never was superior to 80mg/L, except in the first filling period (110mg/L), this concentration of 4CP do not causes biomass inhibition problems. S* was around 30mg/L.

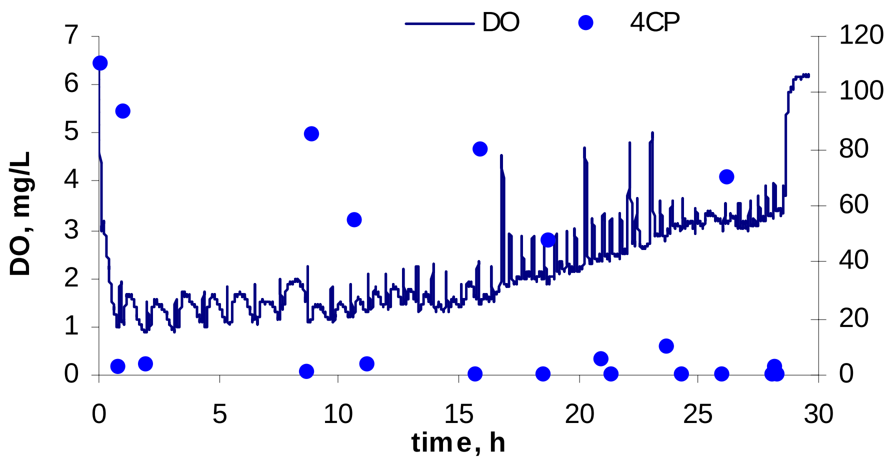
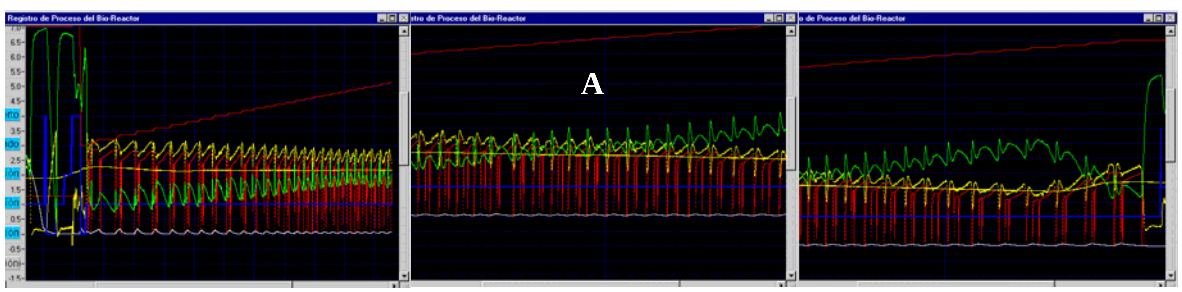


Figure 16. *Behavior of the substrate concentration, measured as 4CP, COD, and DOC during the degradation of 20g 4CP using the ED-TOC strategy*

3.1.5. Degradation of 28g 4CP by the ED-TOC strategy

The degradation of 28g 4CP was made in 42h (the total cycle was 43h), Figure 17 presents the degradation during this cycle. The quantity of 4CP was never superior to 80mg/L, except in the beginning of the cycle, where the concentration was around 130 mg/L). In the subsequent cycles, the maximal concentration filled to the reactor was 43 mg/L. At this point, the reactor was operated around S* (20mg/L 4CP). It is interesting to note that independently of the influent concentration, in this case 7000 mg/L, no inhibition problems of the biomass were observed.



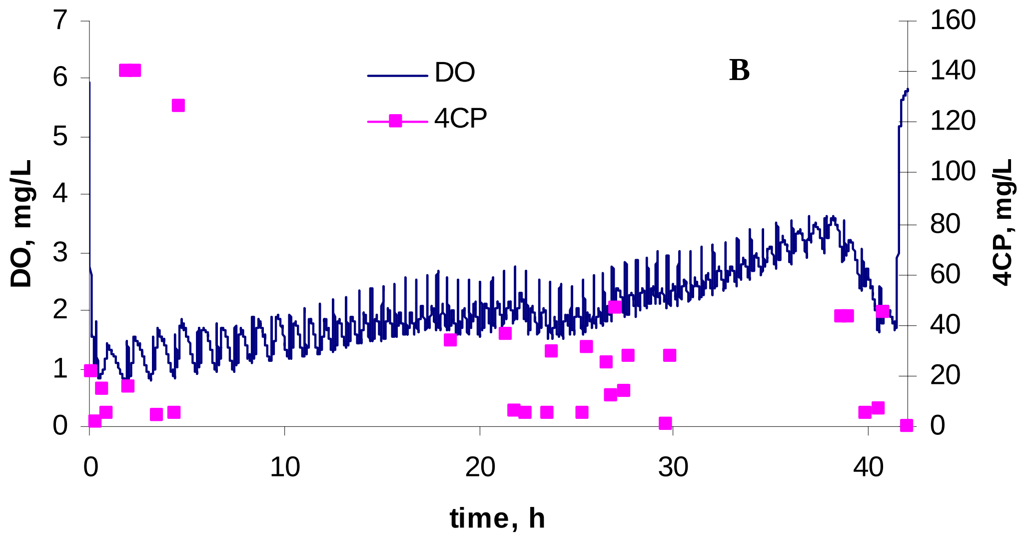


__Figure 17__. A) Screen of the process. B) Behavior of the substrate concentration (4CP) and DO during the degradation of 28g 4CP using the ED-TOC strategy

3.1.5. Comparison of FTC and ED-TOC strategies

With the results obtained it was possible to compare the performances for both strategies. Also, the capacity of the ED-TOC strategy for degrading shock loads of toxic compounds was verified.

The comparison of the strategies showed that the necessary time to degrade the same quantity of 4CP, is lower with the use of the ED-TOC strategy (figure 18). This time for the ED-TOC is lower from 88% to 52% for 1.4g and 28g, respectively. The higher the quantity of 4CP, the lower the degradation time with the ED-TOC strategy.

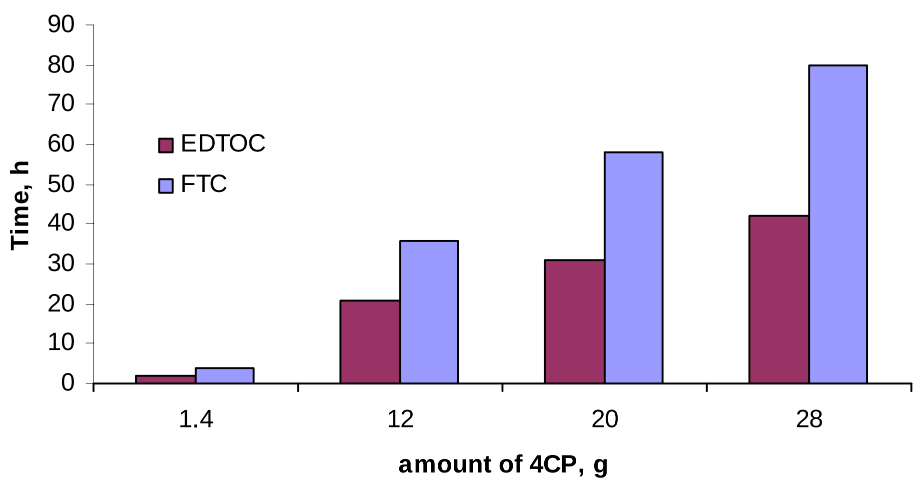


***Figure 18.** Comparison of the time necessary for degrading the same quantity of 4CP by the FTC and ED-TOC strategies*

The specific degradation rate did not show significant differences when comparing both strategies. For FTC strategy the specific degradation rate was 50 mg4CP/gVSS.h, and for ED-TOC it varied between 46 and 50 mg4CP/gVSS-h, for the three studied toxicant amounts. This can be explained because although there exists a great difference in the concentration of the wastewater to degrade (350mg/L for FTC and 3000, 5000 or 7000 mg/L for ED-TOC, by cycle), it does not exist significant differences in the concentration of the water in the reactor (between 50 and 200mg/L), which avoids an inhibition by the concentration of 4CP within the system.

It can be observed that for the ED-TOC strategy the applied load is almost the double (table 1) than that obtained for the FTC strategy. For the degradation of phenols Herzbrun *et al*., (1985) reported a value of 0.26 kgCOD/m^3.d for a pilot scale reactor. Also, Buitrón (1994) reported a value of 1.2 kgCOD/m^3.d for the degradation of 4CP using a strategy similar to the FTC. This way it is demonstrated that it is preferable to use the ED-TOC strategy, since it allows the degradation of loads very superior to the reported in literature.

Table 1. Applied load degrade by the different strategies

4CP, g	**applied load (kgCOD/m^3.d)**	
	FTC (for each cycle)	**ED-TOC**
12		**4.11**
20	**2.52**	**4.80**
28		**4.80**

An important point of comparison is that with FTC strategy it is not possible to degrade influents with concentrations superior to 500mg/L. In addition, it has been observed that inhibition and a total loss of the activity of the microbial consortia is found when a concentration of 1050mg/L is applied to the reactor (Buitrón *et al*., 2003). However, ED-TOC strategy could theoretically degrade any amount of toxic in the influent. In the experiments results it was show that it is possible to degrade an amount of 28g of 4CP, which is equivalent to a concentration in the influent of 7000mg/L of 4CP. This concentration is 10 times superior to the one which would cause a total inhibition using the FTC strategy in the sequential discontinuous reactors.